

MASSIVE FIELD-THEORY APPROACH TO SURFACE CRITICAL BEHAVIOR IN THREE-DIMENSIONAL SYSTEMS

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The massive field-theory approach for studying critical behavior in fixed space dimensions $d < 4$ is extended to systems with surfaces. This enables one to study surface critical behavior directly in dimensions $d < 4$ without having to resort to the ϵ expansion. The approach is elaborated for the representative case of the semi-infinite $|\phi|^4$ n -vector model with a boundary term $\frac{1}{2}c_0 \int_{\partial V} \phi^2$ in the action. To make the theory uv finite in bulk dimensions $3 \leq d < 4$, a renormalization of the surface enhancement c_0 is required in addition to the standard mass renormalization. Adequate normalization conditions for the renormalized theory are given. This theory involves two mass parameter: the usual bulk ‘mass’ (inverse correlation length) m , and the renormalized surface enhancement c . Thus the surface renormalization factors depend on the renormalized coupling constant u and the ratio c/m . The special and ordinary surface transitions correspond to the limits $m \rightarrow 0$ with $c/m \rightarrow 0$ and $c/m \rightarrow \infty$, respectively. It is shown that the surface-enhancement renormalization turns into an additive renormalization in the limit $c/m \rightarrow \infty$. The renormalization factors and exponent functions with $c/m = 0$ and $c/m = \infty$ that are needed to determine the surface critical exponents of the special and ordinary transitions are calculated to two-loop order. The associated series expansions are analyzed by Padé-Borel summation techniques. The resulting numerical estimates for the surface critical exponents are in good agreement with recent Monte Carlo simulations. This also holds for the surface crossover exponent Φ , for which we obtain the values $\Phi(n=0) \simeq 0.52$ and $\Phi(n=1) \simeq 0.54$ considerably lower than the previous ϵ -expansion estimates.

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I. INTRODUCTION

Sparked by the emergence of renormalization group (RG) methods at the beginning of the 1970s, the theory of bulk critical phenomena has undergone a tremendous development in the past 25 years [1–3]. Thanks to a very fruitful interaction with field theory, impressive progress has been achieved both in the theory of bulk critical behavior and in field theory. While the latter has provided a rich variety of powerful tools such as Feynman-graph expansions and renormalized perturbation theory, on which analytical RG approaches could be based, the former has offered a wealth of challenging physical problems and served as a test laboratory for the application of new field-theory techniques.

One popular line of approach that has been extensively used with remarkable success are expansions about the upper critical dimension d^* ($= 4$ for an ordinary bulk critical point) [4]. The advantage of this technique is well known: The computational effort required for calculations to low orders in $\epsilon \equiv d^* - d$ is relatively modest, in particular, if the simplifying features of such elegant schemes as dimensional regularization and minimal subtraction of poles [5] are fully exploited. As a consequence, the calculations can be — and have been [6,7] — pushed to fairly high orders.

A major reason for this computational simplicity is that the calculations can be performed directly for the critical (massless) theory. However, there is a price one must pay. The ϵ expansion involves a double expansion in ϵ and u , the renormalized coupling constant. In making this double expansion one by-passes the problem that the perturbation series of the critical theory in terms of the massless propagator of the free theory is ill-defined for fixed $d < 4$ because of infrared singularities. In the dimensionally regularized theory, these singularities manifest themselves as poles at rational values of ϵ which accumulate at $d = d^*$ as the order of perturbation theory increases [8,9]. Thus the problem of summing these infrared singularities arises. As stressed by Parisi [10], without an additional hypothesis on the

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summation of these singularities, any calculation based on the ϵ expansion and the RG in this perturbative zero-mass scheme does not contain any information about the critical behavior in a fixed dimension $d < d^*$.

In practice, the ϵ expansion often works amazingly well for critical exponents, even if truncated at order ϵ^2 and extrapolated to $d = 3$ in the most naive fashion by setting $\epsilon = 1$. However, quantitatively accurate results require higher orders and sophisticated summation techniques [6,7,11]. The extrapolation problem usually is more severe for other universal quantities such as amplitude ratios¹ or scaling functions. One reason is that the results typically involve (e.g., geometric) factors or functions with an explicit dependence on d . Thus the question arises whether and which of these d -dependent terms should be expanded in ϵ or rather be kept in the extrapolation procedure. As an empirical rule it has been advocated to choose the scale of u in such a fashion that a particular d -dependent geometrical factor is absorbed [13]. From a purely practical point of view, such recipes may well be useful. But they are hardly satisfactory since they neither have a firm theoretical basis we are aware of, nor ensure that all ambiguities of the extrapolation procedure are eliminated in a reliable fashion.

The field-theoretic RG approach based on the ϵ expansion has also been extended [14–19] to, and successfully used in, the study of critical behavior of systems with *surfaces*² [18–20]. In the case of such systems an additional complication may arise: even at low orders of the loop expansion, the perturbative results may involve both geometric factors associated with the d dimensional bulk as well as others coming from the $d - 1$ dimensional boundaries. Hence it may not even be clear how to apply the empirical rule just mentioned.

From a fundamental point of view, approaches that work directly in a *fixed dimension* and therefore *avoid* the ϵ expansion are clearly more attractive. An important one of this kind is the *massive field-theory approach for fixed $d < d^*$* [10,21–28,3]. Its merits are well known: Pushed to sufficiently high orders of perturbation theory and combined with sophisticated series summation techniques, it has produced values of bulk critical exponents [22,23] with an accuracy comparable to that of the most precise ones obtained so far by alternative methods [6,7,11,29,30], as well as a set of amplitude ratios of barely inferior precision [24,25,31]. The method has also been utilized, albeit not to the same level of precision, to determine the universal ratio of correlation-length amplitudes for three-dimensional Ising systems [32], in the analysis of critical behavior in various anisotropic and disordered systems [33–35], partly even in general, non-integer dimensions $2 \leq d < 4$ [36], as well as in studies of three-dimensional ϕ^3 theories describing the percolation transition and the Yang-Lee edge singularity problem [37].

In the present paper (a brief account of which has been given in Ref. [38]), we generalize the massive field-theory approach for fixed $d < d^*$ to the study of critical behavior in *semi-infinite systems*. Such an extension is very desirable, both on account of the general conceptual reasons explained above, and for purely practical purposes. Recently extensive Monte Carlo calculations [39–44] have been performed for three-dimensional Ising models with free surfaces and for the adsorption of polymers on walls³ [45,46,39,43]. For most surface critical exponents these yielded values in reasonable agreement with the ones obtained by setting $\epsilon = 1$ in their ϵ expansion to order ϵ^2 [18]. For the surface crossover exponent Φ [18,20], however, the Monte Carlo estimates turned out to be 20–30% lower. These discrepancies were one of the motives for the present work.

Our analysis is based on the semi-infinite n -vector model, which is the appropriate prototype model for studying surface effects on critical behavior [18]. In Sec. II we briefly recall its definition and provide the necessary background. In Sec. III we give normalization conditions for the massive field theory. Sections IV–VI are devoted to the analysis of the *special* transition. In Sec. IV the general scheme of our approach is explained; then the Callan-Symanzik equations are given and utilized to derive the asymptotic scaling forms of the correlation functions near the multicritical point describing the special transition. After a brief discussion of some general features of perturbation theory, our two-loop results for the RG functions are presented in Sec. V. These are utilized in Section VI to obtain numerical estimates for the values of the surface critical exponents of the special transition in three dimensions by means of Padé analyses and Padé-Borel summation techniques. The *ordinary* transition is treated in Sec. VII. Again, two-loop results are given and exploited to obtain Padé-Borel estimates of its surface critical exponents for $d = 3$. Concluding remarks are reserved for Sec. VIII. Various calculational details are relegated to Appendices A and B.

II. BACKGROUND

¹For a review of results on universal amplitude ratios, see Ref. [12].

²For a review of surface critical phenomena, see Refs. [18] and [20]; for an account of more recent results, see Ref. [19].

³For background and references on polymer adsorption on walls, see Refs. [45] and [46].

A. The model

Let $\phi = (\phi^a(\mathbf{x}))$ be an n -vector field defined on the half-space $V = \mathbb{R}_+^d \equiv \{\mathbf{x} = (\mathbf{r}, z) \in \mathbb{R}^d \mid \mathbf{r} \in \mathbb{R}^{d-1}, z \geq 0\}$ bounded by the plane $z = 0$, which we denote as ∂V . The semi-infinite n -vector model is defined by the Euclidean action [18,19]

$$\mathcal{H}[\phi] = \int_V \left(\frac{1}{2} (\partial_\mu \phi)^2 + \frac{1}{2} m_0^2 \phi^2 + \frac{1}{4!} u_0 |\phi|^4 \right) + \int_{\partial V} \left(\frac{1}{2} c_0 \phi^2 \right). \quad (2.1)$$

Here m_0^2 , u_0 , and c_0 are the bare mass, the bare coupling constant, and the bare surface enhancement⁴, respectively. Adding bulk and surface source terms to the action, we introduce the generating functional

$$\mathcal{Z}[\mathbf{J}, \mathbf{J}_1; K, K_1] = \int \mathcal{D}\phi \exp \left[-\mathcal{H} + \int_V \left(\mathbf{J} \cdot \phi + \frac{1}{2} K \phi^2 \right) + \int_{\partial V} \left(\mathbf{J}_1 \cdot \phi + \frac{1}{2} K_1 \phi^2 \right) \right] \quad (2.2)$$

and the correlation functions

$$\begin{aligned} & G^{(N, M; I, I_1)}(\mathbf{x}_1, \dots, \mathbf{R}_{I_1}) \\ &= \left[\prod_{j=1}^N \frac{\delta}{\delta J^{a_j}(\mathbf{x}_j)} \right] \left[\prod_{k=1}^M \frac{\delta}{\delta J_1^{b_k}(\mathbf{r}_k)} \right] \left[\prod_{l=1}^I \frac{\delta}{\delta K(\mathbf{X}_l)} \right] \left[\prod_{m=1}^{I_1} \frac{\delta}{\delta K_1(\mathbf{R}_m)} \right] \ln \mathcal{Z} \Big|_{J=J_1=K=K_1=0}. \end{aligned} \quad (2.3)$$

For the functions $G^{(N, M; 0, 0)}$ without ϕ^2 -insertions on or off the surface we use the notation $G^{(N, M)}$. The tensorial indices $\{a_j, b_k\}$ will be suppressed whenever no confusion is possible. The ultraviolet (uv) singularities of the theory should be assumed to be regularized by means of a large-momentum cutoff Λ .

We shall also need the (bulk) analogs of these functions for the $|\phi|^4$ theory in the infinite space, i.e., with $V = \mathbb{R}^d$. The easiest way to define these is the usual one where all boundary terms in the action (2.1) and the generating functional (2.2) are dropped, and periodic boundary conditions are chosen. We denote the so-defined bulk analog of $G^{(N, 0; I, 0)}(\{\mathbf{x}_j\}; \{\mathbf{X}_l\})$ as $G_{\text{bulk}}^{(N; I)}(\{\mathbf{x}_j\}; \{\mathbf{X}_l\})$ and introduce their Fourier transforms $\tilde{G}_{\text{bulk}}^{(N; I)}$ through

$$\begin{aligned} & G_{\text{bulk}}^{(N; I)}(\{\mathbf{x}_j\}; \{\mathbf{X}_l\}) \\ &= \int_{\mathbf{q}_1, \dots, \mathbf{Q}_I} \tilde{G}_{\text{bulk}}^{(N; I)}(\{\mathbf{q}_j\}; \{\mathbf{Q}_l\}) e^{i(\sum_j \mathbf{q}_j \mathbf{x}_j + \sum_l \mathbf{Q}_l \mathbf{X}_l)} (2\pi)^d \delta\left(\sum_j \mathbf{q}_j + \sum_l \mathbf{Q}_l\right), \end{aligned} \quad (2.4)$$

where the integral on the right-hand side indicates integrations $\int_{\mathbf{q}} \equiv \int d^d(q/2\pi)$ over all d -dimensional momenta $\mathbf{q}_1, \dots, \mathbf{Q}_I$. For the associated standard bulk vertex functions and their Fourier transforms we use the notation $\Gamma_{\text{bulk}}^{(N; I)}$ and $\tilde{\Gamma}_{\text{bulk}}^{(N; I)}$, respectively.

In the case of our half-space geometry, where translational invariance is restricted to translations *parallel* to the surface, it is appropriate to perform Fourier transformations only with respect to $(d-1)$ -dimensional parallel coordinates. We denote the $(d-1)$ -dimensional parallel momenta associated with the operators $\phi(\mathbf{x} \notin \partial V)$ and $\phi_s \equiv \phi(\mathbf{x} \in \partial V)$ by lower case \mathbf{p} 's, and those associated with the insertions ϕ^2 and ϕ_s^2 by upper case \mathbf{P} 's. Parallel Fourier transforms are indicated by a hat; for example, the pair correlation function in this $\mathbf{p}z$ representation is written as $\hat{G}^{(2, 0)}(\mathbf{p}; z, z')$.

Infinitely far away from the surface all properties must attain their bulk values. Hence the bulk functions $\hat{G}_{\text{bulk}}^{(N; I)}$ can be obtained from $\hat{G}^{(N, 0; I, 0)}$ by letting all $N+I$ perpendicular coordinates $z_j \rightarrow \infty$, keeping all relative coordinates $z_{jk} \equiv z_j - z_k$ fixed:

$$\lim_{z_1, \dots, z_{N+I} \rightarrow \infty} \hat{G}^{(N, 0; I, 0)}(\{\mathbf{p}\}; \{z_j\}) = \hat{G}_{\text{bulk}}^{(N; I)}(\{\mathbf{p}\}; \{z_{jk}\}), \quad (2.5)$$

where $\{\mathbf{p}\}$ here stands for the set of all $N+I$ parallel momenta.

⁴Upon mapping a semi-infinite (lattice) Ising model with ferromagnetic nearest-neighbor interactions of strength K_1 between surface spins and of strength K elsewhere one finds that c_0 decreases as $(K_1 - K)/K$ increases [18]. For simplicity, we shall nevertheless use the term surface enhancement for c_0 , rather than reserving it for $(-c_0)$ or $(-c_0 + \text{const})$.

To proceed, it is necessary to recall a few well-known properties of the model (2.1) [18]. Its phase diagram exhibits a disordered phase (SD/BD), a surface-ordered, bulk-disordered phase (SO/BD), and a surface-ordered, bulk-ordered phase (SO/BO), provided d exceeds the lower critical dimension $d_{\text{SO/BD}}(n)$ for the appearance of a SO/BD phase.⁵

The boundaries between these phases are the lines of surface, ordinary, and extraordinary transitions. They meet at a multicritical point, $(m_0^2, c_0) = (m_{0c}^2, c_0^{\text{sp}})$, called special point and representing the special transition. The ordinary and extraordinary transitions correspond respectively to the portions $c_0 > c_0^{\text{sp}}$ and $c_0 < c_0^{\text{sp}}$ of the line of bulk criticality $m_0^2 = m_{0c}^2$. The line of surface transitions separates the SD/BD from the SO/BD phase. At bulk criticality, we thus have three distinct transitions — the ordinary, special, and extraordinary transition. Of these only the ordinary and special one can be reached from the disordered phase. Since our present analysis is restricted to the disordered phase, only these latter two types of transitions will be considered.

The restriction to the disordered phase simplifies the analysis considerably. One does not have to deal with a nonvanishing, and spatially varying, order-parameter profile $\langle \phi(\mathbf{x}) \rangle$, and the free propagator in the $\mathbf{p}z$ representation takes the relatively simple form

$$\hat{G}(\mathbf{p}; z, z') = \frac{1}{2\kappa_0} \left[e^{-\kappa_0|z-z'|} - \frac{c_0 - \kappa_0}{c_0 + \kappa_0} e^{-\kappa_0(z+z')} \right] \quad (2.6)$$

with

$$\kappa_0 = \sqrt{p^2 + m_0^2}. \quad (2.7)$$

The translation invariant first term on the right-hand side of (2.6) is the free bulk propagator.

The perturbation series of the correlation functions (2.3) in terms of the free propagator (2.6) can be regularized by setting $\hat{G}(\mathbf{p}; z, z') = 0$ for $|\mathbf{p}| > \Lambda$. Whenever we do not use dimensional regularization, the theory is understood to be regularized in this fashion.

B. Ultraviolet singularities for $d < 4$

Let us first discuss the uv singularities of the theory. For bulk dimensions $d = 4 - \epsilon < 4$ the theory is super-renormalizable. Power counting shows [18,17] that the uv singularities of the functions $\hat{G}^{(N,M)}$ can be absorbed through a mass shift

$$m_0^2 = \hat{m}_0^2 + \delta m_0^2 \quad (2.8)$$

and a surface-enhancement shift

$$c_0 = \hat{c}_0 + \delta c_0. \quad (2.9)$$

In order that the $\hat{G}^{(N,M)}$ be finite for $2 \leq d < 4$ when expressed in terms of \hat{m}_0^2 and \hat{c}_0 , the contributions of order u_0^ρ to these shifts must behave as

$$\delta m_0^2 \sim \Lambda^2 (u_0/\Lambda^\epsilon)^\rho \quad (2.10)$$

and

$$\delta c_0 \sim \Lambda (u_0/\Lambda^\epsilon)^\rho \quad (2.11)$$

in the limit $\Lambda \rightarrow \infty$. In contrast to δm_0^2 , which is known to be uv-divergent for $d \geq 2$, the shift δc_0 diverges only for $d \geq 3$.

⁵This lower critical dimension is given by $d_{\text{SO/BD}}(1) = 2$ and $d_{\text{SO/BD}}(n) = 3$ for the Ising case, $n = 1$, and the n -vector case with $n \geq 2$ and $O(n)$ symmetry, respectively. In the presence of surface terms corresponding to an easy-axis spin anisotropy, a SO/BD phase is possible for $n \geq 2$ if $d > 2$. This case, studied elsewhere [47], will not be considered here. The case $d = 3$ with $O(2)$ symmetry of the Hamiltonian is special in that a surface phase with *quasi-long-range order* can appear, a problem which will also not be considered here. We shall also refrain from a discussion of $(d = 2)$ -dimensional n -vector models with noninteger values of n in the range $-2 \leq n \leq 2$ ('loop models' [48]; see, e.g., [49] and its references). However, we shall estimate the surface critical exponents for the $n \rightarrow 0$ case of polymer adsorption [45,46], both for the ordinary and special transition in $d = 3$ dimensions.

C. Poles of the dimensionally regularized theory

As is well-known [8,9,24], if the theory is regularized dimensionally, then the uv singularities of the bulk correlation functions manifest themselves as poles at $\epsilon = 2/k$, with $k \in \mathbb{N}$. These poles can be eliminated by means of an appropriate mass shift $\delta m_0^2(\epsilon)$. We remind that the two-loop graph shown in Fig. 1 yields a contribution of the form

$$-u_0^2 \frac{n+2}{18} m_0^{2-\epsilon} I_2(\epsilon), \quad I_2(\epsilon) \equiv \int_{\mathbf{q}, \mathbf{q}'} \frac{1}{(q^2+1)(q'^2+1) \left[(\mathbf{q} + \mathbf{q}')^2 + 1 \right]}, \quad (2.12)$$

to

$$\tilde{\Gamma}_{\text{bulk}}^{(2)}(q=0) = \chi_{\text{bulk}}^{-1}, \quad (2.13)$$

the inverse of the bulk susceptibility. The integral has a simple pole at $\epsilon = 1$; i. e., $I_2(\epsilon) = R_2(\epsilon)/(\epsilon-1)$, where $R_2(\epsilon)$

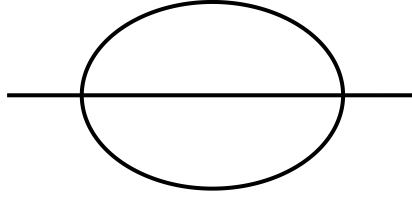


FIG. 1. Two-loop Feynman diagram responsible for the poles in the dimensionally regularized ϕ^4 theory at $d = 3$

is regular at $\epsilon = 1$ and whose value $R_2(1) = 1/32\pi^2$ can be calculated. Removal of the pole is achieved by [24]

$$\delta m_0^2(\epsilon) = u_0^{2/\epsilon} \frac{n+2}{18} \frac{1}{32\pi^2(\epsilon-1)}. \quad (2.14)$$

Expressed in terms of \hat{m}_0^2 and u_0 , the bare bulk functions $\Gamma_{\text{bulk}}^{(N)}$ and $G_{\text{bulk}}^{(N)}$ are then finite at $d = 3$. Yet, they also depend through logarithms on u_0 , and hence in a non-analytic fashion on it.

Not only does this non-analytic behavior carry over to the correlation functions of our semi-infinite theory; owing to the appearance of additional uv (surface) singularities, it shows up already at one-loop order. To see this, consider the surface susceptibility

$$\chi_{11}(m_0, c_0) = \hat{G}^{(0,2)}(p=0; m_0, c_0). \quad (2.15)$$

Its one-loop graph shown in Fig. 2 has a simple pole at $\epsilon = 1$, which can be removed by means of an appropriate choice of δc_0 .

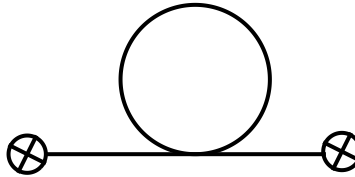


FIG. 2. One-loop graph of the surface susceptibility χ_{11} having a simple pole at $d = 3$. The crossed circles denote points on the surface.

We have

$$\chi_{11}(m_0, c_0)^{-1} = c_0 + m_0 + \frac{n+2}{6} u_0 m_0^{1-\epsilon} \Sigma_1(\epsilon, c_0/m_0) + \mathcal{O}(2\text{-loops}) \quad (2.16)$$

with

$$\begin{aligned}\Sigma_1(\epsilon, \mathbf{c}) &= \int_0^\infty dz e^{-2z} \int_{\mathbf{p}} \frac{1}{2\sqrt{p^2+1}} \left[1 - \frac{\mathbf{c} - \sqrt{p^2+1}}{\mathbf{c} + \sqrt{p^2+1}} e^{-2z\sqrt{p^2+1}} \right] \\ &= J_1(\epsilon) + J_2(\epsilon, \mathbf{c}) + J_3(\epsilon) ,\end{aligned}\tag{2.17}$$

where $\int_{\mathbf{p}} \equiv (1/2\pi)^{d-1} \int d^{d-1}p$,

$$J_1(\epsilon) \equiv \int_{\mathbf{p}} \frac{1}{4\sqrt{p^2+1}} = 2^{-5-\epsilon} \pi^{-2+\epsilon/2} \Gamma\left(-1 + \frac{\epsilon}{2}\right) ,\tag{2.18}$$

$$J_2(\epsilon, \mathbf{c}) \equiv -\frac{\mathbf{c}}{2} \int_{\mathbf{p}} \frac{1}{\sqrt{p^2+1}} \frac{1}{1+\sqrt{p^2+1}} \frac{1}{\mathbf{c} + \sqrt{p^2+1}} ,\tag{2.19}$$

and

$$J_3(\epsilon) \equiv \int_{\mathbf{p}} \frac{1}{4\sqrt{p^2+1}} \frac{1}{1+\sqrt{p^2+1}} = \frac{1}{\epsilon-1} 2^{-3} \pi^{-1+\epsilon/2} \frac{\Gamma(\epsilon)}{\Gamma[(\epsilon+1)/2]} .\tag{2.20}$$

The functions J_1 and J_2 are regular at $\epsilon = 1$; the above-mentioned pole results from J_3 . Upon expansion of the Γ -functions and computation of

$$J_2(1, \mathbf{c}) = \frac{\mathbf{c} \ln 2 - \ln(\mathbf{c}+1)}{8\pi(1-\mathbf{c})} ,\tag{2.21}$$

one arrives at the Laurent expansion

$$\Sigma_1(\epsilon, \mathbf{c}) = \frac{1}{8\pi(\epsilon-1)} + R_1(\mathbf{c}) + \mathcal{O}(\epsilon-1)\tag{2.22}$$

with

$$R_1(\mathbf{c}) = \frac{\mathbf{c} \ln 2 - \ln(\mathbf{c}+1)}{8\pi(1-\mathbf{c})} - \frac{1}{32\pi} - \frac{C_E - \ln \pi}{16\pi} .\tag{2.23}$$

Demanding that the pole be canceled by δc_0 gives

$$\delta c_0(\epsilon) = -u_0^{1/\epsilon} \frac{n+2}{48\pi} \frac{1}{\epsilon-1} .\tag{2.24}$$

Expressed in terms of \hat{c}_0 , \hat{m}_0 , and u_0 , the bare susceptibility is finite at $d = 3$. At the level of our one-loop calculation, one finds

$$\chi_{11}^{-1}|_{\epsilon=1} = \hat{c}_0 + \hat{m}_0 + \frac{n+2}{6} u_0 \left[R_1(\hat{c}_0/\hat{m}_0) - \frac{1}{8\pi} \ln \frac{\hat{m}_0}{u_0} \right] + \mathcal{O}(2\text{-loops}) .\tag{2.25}$$

The critical values $\hat{m}_{0c}^2 = m_{0c}^2 - \delta m_0^2$ and $\hat{c}_0^{\text{sp}} = c_0^{\text{sp}} - \delta c_0$ of \hat{m}_0^2 and \hat{c}_0 pertaining to the special point would have to be determined from the conditions

$$\tilde{\Gamma}_{\text{bulk}}^{(2)}(q=0; m_{0c}^2 = \hat{m}_{0c}^2 + \delta m_0^2) = 0\tag{2.26}$$

and

$$\chi_{11}^{-1}\left(m_{0c} = \sqrt{\hat{m}_{0c}^2 + \delta m_0^2}, c_0^{\text{sp}} = \hat{c}_0^{\text{sp}} + \delta c_0\right) = 0 .\tag{2.27}$$

The former is known to have the form [8]

$$\hat{m}_{0c}^2 = u_0^{2/\epsilon} \hat{\mathcal{M}}(\epsilon) .\tag{2.28}$$

Similarly we have for the latter

$$\hat{c}_0^{\text{sp}} = u_0^{1/\epsilon} \hat{\mathcal{C}}(\epsilon) .\tag{2.29}$$

The reason is that u_0 is the only dimensionful parameter remaining at the special point in the dimensionally regularized theory (with $\Lambda = \infty$ and $\epsilon > 0$). In view of the non-analytic dependence of the susceptibilities on u_0 , it is clear that Symanzik's observation [8] that $\hat{\mathcal{M}}(\epsilon)$ cannot be determined perturbatively carries over to $\hat{\mathcal{C}}(\epsilon)$.

In the next section we describe an appropriate extension of the massive field theory approach that circumvents these difficulties.

III. NORMALIZATION CONDITIONS FOR THE MASSIVE FIELD THEORY

Our aim is to study surface critical behavior at a *bulk critical* point. Therefore, a necessary property we ought to require from our approach is that the bulk critical behavior be treated appropriately. A convenient way to achieve this is to choose it in such a manner that it reduces *for all bulk quantities* to a well-established standard procedure. In our case this will be the conventional one based on normalization conditions (see, e. g., [3,27,28,50,51]). Alternatively, one could choose an approach based on minimal subtraction of poles of the massive theory, as described for the bulk case by Schloms and Dohm [26].

A. Bulk normalization conditions

Starting from the bare bulk vertex functions $\Gamma_{\text{bulk}}^{(N,I)}(; m_0^2, u_0)$, we perform a mass shift

$$m_0^2 = m^2 + \delta m^2(\epsilon) \quad (3.1)$$

and introduce renormalization factors $Z_\phi(u)$, $Z_{\phi^2}(u)$, $Z_u(u)$ (which are uv-finite for $d < 4$) as well as a renormalized dimensionless coupling constant u and renormalized fields such that

$$\phi = [Z_\phi(u)]^{1/2} \phi_{\text{ren}} , \quad \phi^2 = [Z_{\phi^2}(u)]^{-1} [\phi^2]_{\text{ren}} , \quad u_0 = Z_u(u) m^\epsilon u . \quad (3.2)$$

The mass shift and the renormalization factors are fixed through the standard normalization conditions

$$\tilde{\Gamma}_{\text{bulk,ren}}^{(2)}(q; u, m) \Big|_{q=0} = m^2 , \quad (3.3a)$$

$$\frac{\partial}{\partial q^2} \tilde{\Gamma}_{\text{bulk,ren}}^{(2)}(q; u, m) \Big|_{q=0} = 1 , \quad (3.3b)$$

$$\tilde{\Gamma}_{\text{bulk,ren}}^{(2,1)}(\mathbf{q}, \mathbf{Q}; u, m) \Big|_{\mathbf{q}=\mathbf{Q}=0} = 1 , \quad (3.3c)$$

$$\tilde{\Gamma}_{\text{bulk,ren}}^{(4)}(\{\mathbf{q}_i\}; u, m) \Big|_{\{\mathbf{q}_i=0\}} = m^\epsilon u \quad (3.3d)$$

for the renormalized vertex functions

$$\Gamma_{\text{bulk,ren}}^{(N,I)}(\{\mathbf{q}, \mathbf{Q}\}; m, u) = [Z_\phi(u)]^{N/2} [Z_{\phi^2}(u)]^I \Gamma_{\text{bulk}}^{(N,I)}(\{\mathbf{q}, \mathbf{Q}\}; m_0^2, u_0) . \quad (3.4)$$

Since the mass shift is sufficient to absorb the uv singularities of the bare functions $\Gamma_{\text{bulk}}^{(N,I)}$ at $d < 4$, they become uv-finite when expressed in terms of m and u (or m and u_0). The bulk renormalization factors can be written as

$$[Z_\phi(u)]^{-1} = \frac{\partial}{\partial q^2} \tilde{\Gamma}_{\text{bulk}}^{(2)}[q; m_0^2(m, u), u_0(m, u)] \Big|_{q=0} , \quad (3.5a)$$

$$[Z_{\phi^2}(u) Z_\phi(u)]^{-1} = \tilde{\Gamma}_{\text{bulk}}^{(2,1)}[\{\mathbf{0}\}; m_0^2(m, u), u_0(m, u)] , \quad (3.5b)$$

and

$$[Z_u(u) Z_\phi^2(u)]^{-1} = \tilde{\Gamma}_{\text{bulk}}^{(4)}[\{\mathbf{0}\}; m_0^2(m, u), u_0(m, u)] / u_0(m, u) . \quad (3.5c)$$

B. Surface normalization conditions

Consider now the cumulants $G^{(N,M)}$ and $G^{(N,M;I,I_1)}$ of our semi-infinite ϕ^4 model. As we have seen, a surface-enhancement shift δc is required to absorb uv singularities located on the surface. Hence we write

$$c_0 = c + \delta c, \quad (3.6)$$

where c is a renormalized surface enhancement whose precise definition we still have to give.

We also know that the surface operators $\phi_s \equiv \phi|_{z=0}$ and $(\phi_s)^2$ should scale with scaling dimensions that are different from those of their bulk analogs $\phi(\mathbf{x})$ and $[\phi(\mathbf{x})]^2$ with $\mathbf{x} \notin \partial V$. This suggests the introduction of separate renormalization factors for these surface operators, which we do via the relations

$$\phi_s = [Z_\phi Z_1]^{1/2} [\phi_s]_{\text{ren}}, \quad (\phi_s)^2 = [Z_{\phi_s^2}]^{-1} [(\phi_s)^2]_{\text{ren}} \quad (3.7)$$

between the bare and renormalized operators. For the renormalized cumulants we thus have

$$G_{\text{ren}}^{(N,M)}(; m, u, c) = Z_\phi^{-(N+M)/2} Z_1^{-M/2} G^{(N,M)}(; m_0, u_0, c_0) \quad (3.8)$$

and

$$G_{\text{ren}}^{(N,M;I,I_1)}(; m, u, c) = Z_\phi^{-(N+M)/2} Z_1^{-M/2} [Z_{\phi^2}]^I [Z_{\phi_s^2}]^{I_1} G^{(N,M;I,I_1)}(; m_0, u_0, c_0). \quad (3.9)$$

We wish to fix δc and the new renormalization factors Z_1 and $Z_{\phi_s^2}$ by appropriate normalization conditions. To motivate our choice, let us recall the perturbation expansion of the momentum-dependent surface susceptibility $\chi_{11}(p) = \hat{G}^{(0,2)}(p)$ to lowest order:

$$\hat{G}^{(0,2)}(p; m_0, u_0, c_0) = \frac{1}{c_0 + \sqrt{p^2 + m_0^2}} + \mathcal{O}(u_0). \quad (3.10)$$

We choose the normalization conditions such that the associated renormalized susceptibility and its first derivatives with respect to p^2 agree at $p = 0$ with the corresponding zero-loop expressions implied by (3.10), except for the replacements $m_0 \rightarrow m$ and $c_0 \rightarrow c$. This gives

$$\hat{G}_{\text{ren}}^{(0,2)}(p; m, u, c) \Big|_{p=0} = \frac{1}{m + c} \quad (3.11a)$$

and

$$\frac{\partial}{\partial p^2} \hat{G}_{\text{ren}}^{(0,2)}(p; m, u, c) \Big|_{p=0} = -\frac{1}{2m(m+c)^2}. \quad (3.11b)$$

The following condition fixes the normalization of insertions of the surface operator $\frac{1}{2}\phi_s^2$, at zero external momentum:

$$\hat{G}_{\text{ren}}^{(0,2;0,1)}(\mathbf{p}, \mathbf{P}; m, u, c) \Big|_{\mathbf{p}=\mathbf{P}=\mathbf{0}} = (m+c)^{-2}. \quad (3.11c)$$

This choice is motivated by the relation

$$\hat{G}^{(0,2;0,1)}(\{\mathbf{0}\}) = -\frac{\partial}{\partial c_0} \hat{G}^{(0,2)}(0). \quad (3.12)$$

Equation (3.11a) defines the required surface-enhancement shift δc . Together with (3.3a), it ensures that the special point is located at $m = c = 0$. The ordinary transition corresponds to the limit $m \rightarrow 0$ at fixed $c > 0$. In this limit the renormalized surface susceptibility $\chi_{11,\text{ren}} \rightarrow c^{-1}$. Hence the physical meaning of c is that of the inverse of $\chi_{11,\text{ren}}$ at the transition.⁶

⁶Keeping c (and u) fixed while changing m requires, of course, that the bare quantities c_0 (and u_0) be varied with m . When exploiting the Callan-Symanzik equations below, we shall as usual hold these bare quantities fixed while varying m , so that the renormalized quantities u and c become m -dependent.

Equations (3.11b) and (3.11c) specify the renormalization factors Z_1 and $Z_{\phi_s^2}$, respectively, in a similar manner as the bulk normalization conditions (3.3b) and (3.3c) define Z_ϕ and Z_{ϕ^2} . The corresponding expressions are

$$Z_1 Z_\phi = -2m(m+c)^2 \frac{\partial}{\partial p^2} \hat{G}^{(0,2)}[p; m_0(m, u), u_0(m, u), c_0(c, m, u)] \Big|_{p=0} \quad (3.13a)$$

and

$$Z_{\phi_s^2}^{-1} = -[Z_1 Z_\phi]^{-1} (m+c)^2 \frac{\partial}{\partial c_0} \hat{G}^{(0,2)}[0; m_0(m, u), u_0(m, u), c_0] \Big|_{c_0=c_0(c, m, u)} . \quad (3.13b)$$

The above sets of normalization conditions (3.3a)–(3.3d) and (3.11a)–(3.11c) define m_0^2 , u_0 , Z_ϕ , Z_{ϕ^2} , c_0 , Z_1 , and $Z_{\phi_s^2}$ as functions of m , u , c , and Λ . All Z factors have finite $\Lambda \rightarrow \infty$ limits in the $d < 4$ case considered here.

For simplicity, we consider the $\Lambda = \infty$ limit in the sequel. In our calculations described below we actually took $\Lambda = \infty$ from the outset, employing dimensional regularization. In this limit the bulk Z factors Z_ϕ , Z_{ϕ^2} , and Z_u become functions of the single dimensionless variable u . On the other hand, the above choice of normalization conditions (3.11a)–(3.11c) implies that the surface Z factors Z_1 and $Z_{\phi_s^2}$ depend on both u and the dimensionless ratio c/m .

In a full investigation of the crossover from the surface critical behavior characteristic of the special transition (for $c/m \ll 1$) to that of the ordinary transition (for $c/m \gg 1$), it would be essential to carry along the dependence on the variable c/m . However, our main objective in the present work is the calculation of the surface critical exponents of the special and ordinary transitions. To this end, a study of the critical behavior in the asymptotic limits $c/m \rightarrow 0$ and $c/m \rightarrow \infty$ is sufficient. As it turns out, there exist convenient procedures (see [38] and below) which permit one to focus directly on these limits, avoiding the need to keep track of the detailed dependence on c/m .

IV. SPECIAL TRANSITION

Let us first consider the case of the *special* transition. In order to reach the corresponding multicritical point, we can safely set $c = 0$. This does not cause any problems in the theory provided the surface-enhancement renormalization has been performed. The desired critical behavior at the special transition can then be obtained by studying the massless limit of the resulting massive $c = 0$ theory along lines analogous to those usually followed in the bulk case. It follows that the asymptotic critical behavior at this transition is described by the renormalized theory with the coupling constant u taken at u^* , its value at the infrared-stable fixed point (and c set to zero).

A. Normalization conditions at the multicritical point

For $c = 0$ the normalization conditions (3.11a)–(3.11c) simplify. The $c = 0$ analog of (3.11a) fixes the critical value c_0^{sp} of c_0 . Expressed in terms of renormalized variables, it takes the form $c_0^{\text{sp}} = m f_\epsilon(u)$ in the dimensionally regularized theory. Equations (3.13a) and (3.13b) become

$$Z_1^{\text{sp}}(u) Z_\phi(u) = -2m^3 \frac{\partial}{\partial p^2} \hat{G}^{(0,2)}[p; m_0(m, u), u_0(m, u), c_0^{\text{sp}}(m, u)] \Big|_{p=0} , \quad (4.1a)$$

$$\left[Z_{\phi_s^2}^{\text{sp}}(u) \right]^{-1} = -m^2 [Z_1^{\text{sp}}(u) Z_\phi(u)]^{-1} \frac{\partial}{\partial c_0} \hat{G}^{(0,2)}[0; m_0(m, u), u_0(m, u), c_0] \Big|_{c_0=c_0^{\text{sp}}} , \quad (4.1b)$$

specifying renormalization factors $Z_1^{\text{sp}}(u) \equiv Z_1(u, c/m = 0)$ and $Z_{\phi_s^2}^{\text{sp}}(u) \equiv Z_{\phi_s^2}(u, c/m = 0)$ appropriate for the analysis of the special transition. These renormalization factors enter the relations (3.8) between the bare and renormalized correlation functions $G^{(N,M)}$ for $c = 0$,

$$G_{\text{ren,sp}}^{(N,M)}(; m, u) = Z_\phi^{-(N+M)/2} (Z_1^{\text{sp}})^{-M/2} G^{(N,M)}(; m_0, u_0, c_0^{\text{sp}}) , \quad (4.2)$$

and the corresponding $c = 0$ analogs of the relations (3.9) for $G^{(N,M;I,I_1)}$.

B. Callan-Symanzik equations

By varying m at fixed u_0 and c_0^{sp} , the Callan-Symanzik (CS) equations (cf. Refs. [3,27,28]) of the correlation functions $G_{\text{ren,sp}}^{(N,M)}$ can be derived in a straightforward way. They read

$$\left[m \frac{\partial}{\partial m} + \beta(u) \frac{\partial}{\partial u} + \frac{N+M}{2} \eta_\phi(u) + \frac{M}{2} \eta_1^{\text{sp}}(u) \right] G_{\text{ren,sp}}^{(N,M)}(; m, u) = \Delta G_{\text{ren}}, \quad (4.3a)$$

with

$$\Delta G_{\text{ren}} \equiv -[2 - \eta_\phi(u)] m^2 \int_V d^d X G_{\text{ren,sp}}^{(N,M;1,0)}(; m, u), \quad (4.3b)$$

where the integration is over the position \mathbf{X} of the inserted ϕ^2 operator.

The RG functions appearing here are the usual bulk functions

$$\beta(u) = m \frac{\partial}{\partial m} \Big|_0 u \quad (4.4a)$$

and

$$\eta_\phi(u) = m \frac{\partial}{\partial m} \Big|_0 \ln Z_\phi(u) = \beta(u) \frac{d \ln Z_\phi(u)}{du}, \quad (4.4b)$$

and the additional, surface-related function

$$\eta_1^{\text{sp}}(u) = m \frac{\partial}{\partial m} \Big|_0 \ln Z_1^{\text{sp}}(u) = \beta(u) \frac{d \ln Z_1^{\text{sp}}(u)}{du}, \quad (4.4c)$$

where $|_0$ indicates that the derivatives are taken at fixed bare coupling constant and surface enhancement (and cutoff Λ).

Just as in the bulk case, and as could be corroborated by means of a short-distance expansion, the right-hand side of (4.3a), ΔG_{ren} , should be negligible in the critical regime. The resulting homogeneous equations can be integrated in a standard fashion.

In order to identify the crossover exponent Φ we must also consider deviations $\Delta c_0 \equiv c_0 - c_0^{\text{sp}}$ from the multicritical point. We use the expansion

$$G^{(N,M)}(; m_0, u_0, c_0) = \sum_{I_1=0}^{\infty} \frac{(-\Delta c_0)^{I_1}}{I_1!} \underbrace{\int_{\partial V} \dots \int_{\partial V}}_{I_1} G^{(N,M;0,I_1)}(; m_0, u_0, c_0^{\text{sp}}), \quad (4.5)$$

where the integrations $\int_{\partial V}$ are over the positions of the I_1 inserted ϕ_s^2 operators. No infrared problems arise here because the massive theory is used.

Expressing the right-hand side in terms of renormalized functions and the renormalized variable

$$\Delta c \equiv \left[Z_{\phi_s^2}^{\text{sp}}(u) \right]^{-1} \Delta c_0 \quad (4.6)$$

gives

$$Z_\phi^{-(N+M)/2} (Z_1^{\text{sp}})^{-M/2} G^{(N,M)}(; m_0, u_0, c_0) = \sum_{I_1=0}^{\infty} \frac{(-\Delta c)^{I_1}}{I_1!} \underbrace{\int_{\partial V} \dots \int_{\partial V}}_{I_1} G_{\text{ren,sp}}^{(N,M;0,I_1)}(; m, u). \quad (4.7)$$

Hence

$$G_{\text{ren}}^{(N,M)}(; m, u, \Delta c) \equiv [Z_\phi(u)]^{-(N+M)/2} [Z_1^{\text{sp}}(u)]^{-M/2} G^{(N,M)}(; m_0, u_0, c_0) \quad (4.8)$$

are well-defined renormalized functions.⁷ Since they depend on the additional dimensionless variable

$$c \equiv \Delta c/m , \quad (4.9)$$

their RG equations are analogous to, but differ from, (4.3a) through the replacement

$$m \frac{\partial}{\partial m} + \beta(u) \frac{\partial}{\partial u} \longrightarrow m \frac{\partial}{\partial m} + \beta(u) \frac{\partial}{\partial u} - [1 + \eta_c^{\text{sp}}(u)] c \frac{\partial}{\partial c} , \quad (4.10)$$

where

$$\eta_c^{\text{sp}}(u) = m \frac{\partial}{\partial m} \bigg|_0 \ln Z_{\phi_s^2}^{\text{sp}}(u) = \beta(u) \frac{d}{du} \ln Z_{\phi_s^2}^{\text{sp}}(u) . \quad (4.11)$$

C. Scaling behavior near the multicritical point

The CS equations given in the preceding subsection can be utilized in a familiar fashion to derive the asymptotic scaling forms of the correlation functions near the multicritical point. A detailed exposition of the derivation of scale invariance and universality of bulk vertex functions from the CS equations may be found, for example, in [52] or elsewhere [3]. Since in the present case a completely analogous line of reasoning can be followed, we can be brief. In particular, we shall avoid carrying along the various non-universal constants (metric factors setting the scales of the relevant bulk and surface scaling fields), as would be necessary for an explicit derivation of four-scale-factor universality [53] within the present massive RG framework.

We shall need the familiar dependence

$$m_0^2 - m_{0c}^2 \sim \tau \quad (4.12)$$

of the bare mass on $\tau \equiv (T - T_c)/T_c$, valid for small deviations from its critical value m_{0c}^2 . We also recall that m , which is nothing else than the inverse of the (second-moment) bulk correlation length ξ , behaves as

$$m \sim (m_0^2 - m_{0c}^2)^\nu \quad (4.13)$$

near criticality, with

$$\nu = [2 + \eta_{\phi^2}^*]^{-1} , \quad (4.14)$$

where $\eta_{\phi^2}^*$ denotes the value of the function

$$\eta_{\phi^2}(u) = m \frac{\partial}{\partial m} \bigg|_0 \ln Z_{\phi^2}(u) = \beta(u) \frac{d \ln Z_{\phi^2}(u)}{du} , \quad (4.15)$$

at the infrared-stable zero u^* of $\beta(u)$.

Integration of (4.4a), (4.4b), (4.4c), and (4.11) gives the asymptotic dependencies

$$Z_\phi \sim (u - u^*)^{\eta/\omega} \sim m^\eta , \quad (4.16)$$

$$Z_1^{\text{sp}} \sim (u - u^*)^{\eta_1^{\text{sp}}(u^*)/\omega} \sim m^{\eta_1^{\text{sp}}(u^*)} , \quad (4.17)$$

and

$$Z_c^{\text{sp}} \sim (u - u^*)^{\eta_c^{\text{sp}}(u^*)/\omega} \sim m^{\eta_c^{\text{sp}}(u^*)} \quad (4.18)$$

⁷These should be distinguished from the previously defined c -dependent renormalized functions, which were related to the bare ones via c -dependent renormalization factors.

for $u \rightarrow u^*$ or $m \rightarrow 0$. As usual, $\omega = \beta'(u^*)$ and $\eta \equiv \eta_\phi(u^*)$. Equation (4.18) can be substituted into (4.6) and (4.9) to obtain

$$\Delta c \sim m^{-\eta_c^{\text{sp}}(u^*)} \Delta c_0, \quad c \sim m^{-[1+\eta_c^{\text{sp}}(u^*)]} \Delta c_0. \quad (4.19)$$

From the latter result we read off the scaling variable $\tau^{-\Phi} \Delta c_0$ with the crossover exponent

$$\Phi = \nu[1 + \eta_c^{\text{sp}}(u^*)]. \quad (4.20)$$

Using these results, one easily sees that the CS equations of Sec. IV B yield the following asymptotic scaling forms of the correlation functions near the multicritical point:

$$G^{(N,M)}(\mathbf{x}, \mathbf{r}; m_0, u_0, c_0) \sim m^{(N\beta + M\beta_1^{\text{sp}})/\nu} \Psi^{(N,M)}\left(m\mathbf{x}, m\mathbf{r}, m^{-\Phi/\nu} \Delta c_0\right). \quad (4.21)$$

Here β and β_1^{sp} are standard bulk and surface exponents. The latter is related to the usual surface correlation exponent η_{\parallel} via the scaling law

$$\beta_1 = \frac{\nu}{2} (d - 2 + \eta_{\parallel}), \quad (4.22)$$

where η_{\parallel} in the present case of the special transition is given by

$$\eta_{\parallel}^{\text{sp}} = \eta + \eta_1^{\text{sp}}(u^*). \quad (4.23)$$

V. PERTURBATION THEORY

We now turn to the explicit calculation of the surface renormalization factors Z_1^{sp} and $Z_{\phi_s}^{\text{sp}}$ and of their associated exponent functions η_1^{sp} and η_c^{sp} . In the one-loop approximation, this will be carried out for general space dimensions $d < 4$. However, in our two-loop calculations we shall restrict ourselves to the case $d = 3$.

A. General Features

The normalization conditions (3.11a), (3.11b), and (3.11c) we have chosen to fix the surface counterterms all determine properties of the renormalized surface susceptibility $\hat{G}_{\text{ren}}^{(0,2)}(p; m, u, c)$. For calculational purposes it is more convenient to express these conditions in terms of its bare inverse $1/\hat{G}^{(0,2)}(p)$. From (3.11a) we find

$$Z_1 Z_\phi \left[\hat{G}^{(0,2)}(0; m_0, u_0, c_0) \right]^{-1} = m + c. \quad (5.1a)$$

Utilizing this, (3.11b) becomes

$$\frac{\partial}{\partial p^2} \left[\hat{G}_{\text{ren}}^{(0,2)}(p; m, u, c) \right]^{-1} \Big|_{p=0} = \frac{1}{2m}, \quad (5.1b)$$

which shows that expression (3.13a) for $Z_1 Z_\phi$ can be cast in the equivalent form

$$(Z_1 Z_\phi)^{-1} = 2m \frac{\partial}{\partial p^2} \left[\hat{G}^{(0,2)}(p) \right]^{-1} \Big|_{p=0} = \lim_{p \rightarrow 0} \frac{m}{p} \frac{\partial}{\partial p} \left[\hat{G}^{(0,2)}(p) \right]^{-1}. \quad (5.2a)$$

Likewise (3.13b) can be rewritten as

$$Z_{\phi_s}^{-1} = Z_1 Z_\phi \frac{\partial}{\partial c_0} \left[\hat{G}^{(0,2)}(p=0) \right]^{-1}. \quad (5.2b)$$

It is useful to decompose the above inverse surface susceptibility into its free part, which is $[\hat{G}(\mathbf{p}; 0, 0)]^{-1} = c_0 + \kappa_0$ according to (2.6), and a remainder due to perturbative corrections. Thus we write

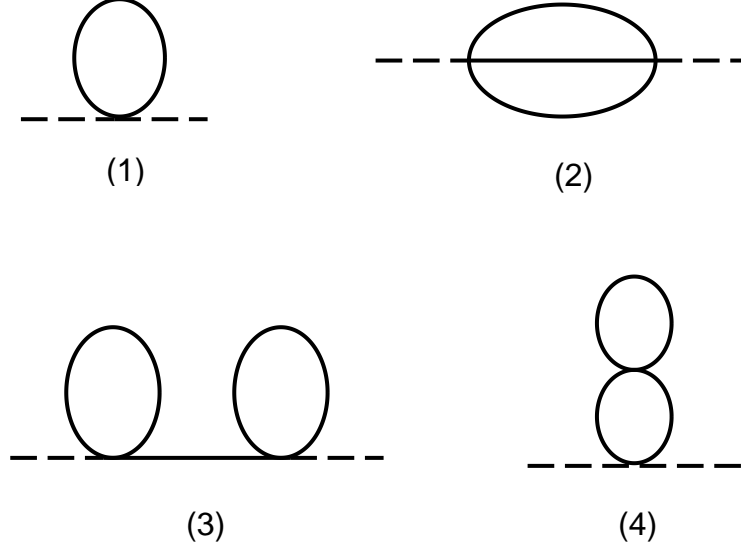


FIG. 3. Feynman graphs to two-loop order of the nominator $\hat{g}^T \hat{T} \hat{g}$ of the quantity $\hat{\sigma}_0(p)$ in (5.5). Full lines denote the free propagator (2.6), dashed ones the reduced propagator (5.6).

$$\left[\hat{G}^{(0,2)}(p) \right]^{-1} = c_0 + \kappa_0 - \hat{\sigma}_0(p). \quad (5.3)$$

To compute $\hat{\sigma}_0$, we start from the following representation of the full propagator between two surface points in terms of Σ , the usual ‘self-energy’:

$$G^{(0,2)} = {}_s|G|_s + {}_s|GTG|_s, \quad T = \Sigma (1 - G\Sigma)^{-1} \quad (5.4)$$

Here ${}_s|$ and $|_s$ indicate that the left and right points are located on the surface, respectively. A straightforward calculation yields

$$\hat{\sigma}_0(p) = \frac{\hat{g}^T \hat{T} \hat{g}}{1 + {}_s|\hat{G}|_s \hat{g}^T \hat{T} \hat{g}} = \hat{g}^T \hat{\Sigma} \hat{g} + \hat{g}^T \hat{\Sigma} \hat{G} \hat{\Sigma} \hat{g} - {}_s|G|_s \left(\hat{g}^T \hat{\Sigma} \hat{g} \right)^2 + \mathcal{O}(\hat{\Sigma}^3), \quad (5.5)$$

where \hat{g} is a column vector whose components represent the reduced propagator

$$\hat{g}(p; z) \equiv (c_0 + \kappa_0) \hat{G}(p; z, 0) = e^{-\kappa_0 z}, \quad (5.6)$$

and \hat{g}^T is its transpose.

The one-loop and two-loop contributions to $\hat{\sigma}_0$ originating from the first two terms on the right-hand side of (5.5) are depicted in Fig. 3. Denoting the one from the graph labeled “(i)” by $C_i(p)$, we have

$$\hat{\sigma}_0(p) = \sum_{i=1}^4 C_i(p) - \frac{[C_1(p)]^2}{c_0 + \kappa_0} + \mathcal{O}(u_0^3), \quad (5.7)$$

where the term $\propto C_1^2$ results from the last one in (5.5).

B. One-Loop Approximation

We now specialize to the case $c = 0$. Upon using the above results together with those presented in Appendix A, one can easily perform a one-loop calculation of the renormalization functions for general dimensions $d < 4$. Following Ref. [21], let us introduce a rescaled renormalized coupling constant \tilde{u} through

$$u = b_n(d) \tilde{u}, \quad b_n(d) = \frac{6}{n+8} \frac{(4\pi)^{d/2}}{\Gamma(\epsilon/2)}. \quad (5.8)$$

The advantage of this choice is that the expansion to order \tilde{u}^2 of the associated beta function $\tilde{\beta} = \beta \partial \tilde{u} / \partial u$ takes the simple form

$$\tilde{\beta}(\tilde{u}) = -\tilde{u}(1 - \tilde{u}) + \mathcal{O}(\tilde{u}^3) . \quad (5.9)$$

Our results for the two surface renormalization factors of interest then read

$$Z_1^{\text{sp}} = 1 + \frac{n+2}{n+8} \frac{\tilde{u}}{1+\epsilon} + \mathcal{O}(\tilde{u}^2) \quad (5.10a)$$

and

$$Z_{\phi_s^2}^{\text{sp}} = 1 - \frac{n+2}{n+8} \frac{1}{1+\epsilon} \left[1 - 2^{\frac{1+\epsilon}{2}} {}_2F_1\left(\frac{3-\epsilon}{2}, \frac{1+\epsilon}{2}; \frac{3+\epsilon}{2}; \frac{1}{2}\right) \right] \tilde{u} + \mathcal{O}(\tilde{u}^2) , \quad (5.10b)$$

where ${}_2F_1$ is the hypergeometric function [54]. Substituting these power series into (4.4c) and (4.11) gives

$$\eta_1^{\text{sp}}(u) \equiv \tilde{\eta}_1^{\text{sp}}(\tilde{u}) = -\frac{n+2}{n+8} \frac{\epsilon}{1+\epsilon} \tilde{u} + \mathcal{O}(\tilde{u}^2) , \quad (5.11a)$$

$$\eta_c^{\text{sp}}(u) \equiv \tilde{\eta}_c^{\text{sp}}(\tilde{u}) = \frac{n+2}{n+8} \frac{\epsilon}{1+\epsilon} \left[1 - 2^{\frac{1+\epsilon}{2}} {}_2F_1\left(\frac{3-\epsilon}{2}, \frac{1+\epsilon}{2}; \frac{3+\epsilon}{2}; \frac{1}{2}\right) \right] \tilde{u} + \mathcal{O}(\tilde{u}^2) . \quad (5.11b)$$

As a consistency check one can compute the pole parts (PP) of the Laurent expansion of the above renormalization factors at $\epsilon = 0$. One finds

$$\text{PP}_{\epsilon=0} [Z_1^{\text{sp}} - 1] = \frac{n+2}{3\epsilon} \frac{u}{16\pi^2} + \mathcal{O}(u^2) \quad (5.12a)$$

$$= \text{PP}_{\epsilon=0} [Z_{\phi_s^2}^{\text{sp}} - 1] + \mathcal{O}(u^2) . \quad (5.12b)$$

As it should, this is in conformity with the one-loop terms (of the two-loop results) of Ref. [16], obtained by means of the usual scheme of minimal subtraction of poles at $d = 4$ for the massless theory in $4 - \epsilon$ dimensions.⁸ Accordingly we also recover the $\mathcal{O}(u)$ expressions for the exponents functions η_1 and η_c of Ref. [16] in the limit $\epsilon \rightarrow 0^+$:

$$\lim_{\epsilon \rightarrow 0^+} \eta_1^{\text{sp}}(u) = -\frac{n+2}{3} \frac{u}{16\pi^2} + \mathcal{O}(u^2) = \lim_{\epsilon \rightarrow 0^+} \eta_c^{\text{sp}}(u) + \mathcal{O}(u^2) . \quad (5.13)$$

From (5.9) one reads off the value $\hat{u}^* = 1$ in this one-loop approximation. Upon inserting this into (5.11), we get

$$\eta_1^{\text{sp}}(u^*) = -\frac{n+2}{n+8} \frac{\epsilon}{1+\epsilon} + \mathcal{O}(2\text{-loop}) = \eta_{\parallel}^{\text{sp}} + \mathcal{O}(2\text{-loop}) \quad (5.14a)$$

and

$$\eta_c^{\text{sp}}(u^*) = \frac{n+2}{n+8} \frac{\epsilon}{1+\epsilon} \left[1 - 2^{\frac{1+\epsilon}{2}} {}_2F_1\left(\frac{3-\epsilon}{2}, \frac{1+\epsilon}{2}; \frac{3+\epsilon}{2}; \frac{1}{2}\right) \right] + \mathcal{O}(2\text{-loop}) . \quad (5.14b)$$

The reader may check that the Taylor expansion of these exponents to first order in ϵ reproduces the known results (see Refs. [16,18] and references therein).

If we use (5.14a) and (5.14b) to estimate their values for $d = 3$, we find

$$\eta_1^{\text{sp}}(n=0) = \eta_{\parallel}^{\text{sp}}(n=0) = -\frac{1}{8} \simeq -0.13 , \quad (5.15a)$$

$$\eta_1^{\text{sp}}(n=1) = \eta_{\parallel}^{\text{sp}}(n=1) = -\frac{1}{6} \simeq -0.17 , \quad (5.15b)$$

⁸Since in Refs. [16] and [18] a factor $2^d \pi^{d/2}$ was absorbed in the renormalized coupling constant, the quantity $u/16\pi^2$ here takes the place of the variable u of these references.

and

$$\eta_c^{\text{sp}}(n=0) = \frac{1}{8} (1 - 4 \ln 2) \simeq -0.22 , \quad (5.16a)$$

$$\eta_c^{\text{sp}}(n=1) = \frac{1}{6} (1 - 4 \ln 2) \simeq -0.30 . \quad (5.16b)$$

Amazingly, the estimates (5.15) of this simple calculation turn out to be among the best ones for $\eta_{\parallel}^{\text{sp}}$ resulting from our much more involved two-loop calculations (see Tables I and II). On the other hand, our best two-loop estimates for η_c^{sp} differ appreciably from those listed in (5.16).

C. Two-Loop Approximation

At two-loop order we restrict ourselves to the case $d = 3$. Details of the calculation may be found in Appendix A. Here we just quote the final results. They read

$$Z_1^{\text{sp}} Z_{\phi} = 1 + \frac{n+2}{2(n+8)} \tilde{u} - \frac{12(n+2)}{(n+8)^2} \left[A - \frac{n+2}{12} (1 - \ln 2) \ln 2 - \frac{n+14}{48} \right] \tilde{u}^2 + \mathcal{O}(\tilde{u}^3) , \quad (5.17a)$$

$$\begin{aligned} Z_{\phi_s^2}^{\text{sp}} = 1 + \frac{n+2}{n+8} \left(2 \ln 2 - \frac{1}{2} \right) \tilde{u} \\ + \frac{12(n+2)}{(n+8)^2} \left[A - B - \frac{n}{2} \ln 2 + \frac{n+2}{2} \ln^2 2 + \frac{2n+1}{12} \right] \tilde{u}^2 + \mathcal{O}(\tilde{u}^3) , \end{aligned} \quad (5.17b)$$

$$\begin{aligned} \eta_{\parallel}^{\text{sp}}(\tilde{u}) = -\frac{n+2}{2(n+8)} \tilde{u} + \frac{12(n+2)}{(n+8)^2} \left[2A - \frac{n+2}{6} (1 - \ln 2) \ln 2 + \frac{n-10}{48} \right] \tilde{u}^2 \\ + \mathcal{O}(\tilde{u}^3) , \end{aligned} \quad (5.18a)$$

and

$$\begin{aligned} \eta_c^{\text{sp}}(\tilde{u}) = -\frac{n+2}{n+8} \left(2 \ln 2 - \frac{1}{2} \right) \tilde{u} - \frac{24(n+2)}{(n+8)^2} \left[A - B - \frac{n+1}{2} \ln 2 \right. \\ \left. + \frac{n+2}{3} \ln^2 2 + \frac{17n+22}{96} \right] \tilde{u}^2 + \mathcal{O}(\tilde{u}^3) , \end{aligned} \quad (5.18b)$$

where A and B are integrals originating from the two-loop graph (2) of Fig. 3 whose values

$$A \simeq 0.202428 \quad (5.19)$$

and

$$B \simeq 0.678061 \quad (5.20)$$

we have determined by numerical means (cf. Appendix A).

VI. SURFACE CRITICAL EXPONENTS OF THE SPECIAL TRANSITION

We shall now discuss how the above perturbative results can be utilized to estimate the surface critical exponents of the special transition. Our starting point are the series expansions of these exponents in powers of \tilde{u} , which are implied by (5.18a) and (5.18b). To generate these series, we substitute the expansion (5.18a) for $\eta_{\parallel}^{\text{sp}}$ into the following well-known scaling-law expressions for surface exponents:

$$\Delta_1 = \frac{\nu}{2} (d - \eta_{\parallel}) , \quad (6.1a)$$

$$\eta_{\perp} = \frac{\eta + \eta_{\parallel}}{2} , \quad (6.1b)$$

$$\beta_1 = \frac{\nu}{2} (d - 2 + \eta_{\parallel}) , \quad (6.1c)$$

$$\gamma_{11} = \nu (1 - \eta_{\parallel}) , \quad (6.1d)$$

$$\gamma_1 = \nu (2 - \eta_{\perp}) , \quad (6.1e)$$

$$\delta_1 = \frac{\Delta}{\beta_1} = \frac{d + 2 - \eta}{d - 2 + \eta_{\parallel}} , \quad (6.1f)$$

$$\delta_{11} = \frac{\Delta_1}{\beta_1} = \frac{d - \eta_{\parallel}}{d - 2 + \eta_{\parallel}} . \quad (6.1g)$$

These scaling relations hold for the surface critical exponents of the ordinary transition as well; therefore, we have omitted the superscript “sp”. We also need the expansions of the bulk exponents ν and η . To the required order in \tilde{u}^* , they read for the case $d = 3$:

$$\nu(d=3, n) = \frac{1}{2} + \frac{n+2}{4(n+8)} \tilde{u}^* + \frac{(n+2)(27n-38)}{216(n+8)^2} (\tilde{u}^*)^2 + \mathcal{O}[(\tilde{u}^*)^3] \quad (6.2a)$$

and

$$\eta(d=3, n) = \frac{8(n+2)}{27(n+8)^2} (\tilde{u}^*)^2 + \mathcal{O}[(\tilde{u}^*)^3] . \quad (6.2b)$$

We shall also consider the exponents

$$\alpha_1^{\text{sp}} = \alpha + \nu - 1 + \Phi = 1 - \nu [d - 2 - \eta_c^{\text{sp}}(u^*)] \quad (6.3a)$$

and

$$\alpha_{11}^{\text{sp}} = \alpha + \nu - 2 + 2\Phi = -\nu [d - 3 - 2\eta_c^{\text{sp}}(u^*)] \quad (6.3b)$$

of the layer and local specific heats $C_1(T)$ and $C_{11}(T)$, respectively [18]. To obtain the expressions on the extreme right-hand side, we have substituted (4.20) for Φ and used the hyperscaling relation $\alpha = 2 - d\nu$.

For each one of these surface exponents we arrive at an expansion of the form

$$f(\tilde{u}^*) = \sum_{k=0}^{\infty} f_k (\tilde{u}^*)^k = f_0 + f_1 \tilde{u}^* + f_2 (\tilde{u}^*)^2 + \mathcal{O}[(\tilde{u}^*)^3] . \quad (6.4)$$

As is known from the much studied bulk case (for background and references, see, e.g., [3]), such series are *asymptotic*; they have *zero radius of convergence*. The reason for this is that the coefficients f_k grow proportional to $k!$ as $k \rightarrow \infty$; more precisely, their large- k behavior typically can be written as $f_k \approx \mathcal{C} k! k^{b-1} \mathcal{A}^{-k}$, where the factor $k!$ basically reflects the enormous growth of the number of diagrams contributing at a given order of the loop expansion. We expect that these features will carry over to the power series of surface quantities considered here. The large-order behavior of their coefficients and the values of the numbers \mathcal{A} , b , and \mathcal{C} should be obtainable by means of an appropriate extension of the instanton calculus utilized in the case of the $|\phi|^4$ bulk theory. Furthermore, in view of the rigorously established Borel summability of the $d = 3$ dimensional $|\phi|^4$ model [55], we may be confident that these series are Borel summable.

In order to obtain meaningful numerical estimates from the above series expansions for surface critical exponents, we must invoke appropriate and sufficiently powerful summation techniques. The simplest procedure is to construct the table of Padé approximants [56]. This works well if successive elements S_N , S_{N+1} of the sequence of partial sums $S_N(\tilde{u}^*) \equiv \sum_{k=0}^N f_k (\tilde{u}^*)^k$ vary little at low orders of N . A better and more sophisticated one is the Padé-Borel

method used in Ref. [21]. At the order of perturbation theory we are going to use it here, this involves the analytic continuation of the Borel transform

$$B_f(\tilde{u}^*) \equiv \sum_{k=0}^{\infty} \frac{f_k}{k!} (\tilde{u}^*)^k \quad (6.5)$$

by a [1/1] Padé approximant.

Our estimates given in Tables I–IV were produced as follows. For each exponent f , we rearranged the expansion as $f/f_0 \equiv M_f = 1 + (f_1/f_0)\tilde{u}^* + (f_2/f_0)(\tilde{u}^*)^2$ or $f + (1 - f_0) \equiv M_f = 1 + f_1\tilde{u}^* + f_2(\tilde{u}^*)^2$, depending on whether $|f_0| > 1$ or $|f_0| < 1$, respectively. Then Padé approximants of the type indicated in Tables I–IV were constructed for the so-defined modified quantities M_f , and [1/1] Padé approximants for their Borel transforms. For consistency reasons, these approximants were evaluated using the values of $\tilde{u}^*(d, n)$ one gets from the Padé-Borel resummed beta functions $\tilde{\beta}(\tilde{u})$ at this two-loop order, namely⁹ [21,57]

$$\tilde{u}^*(d=3, n=0) = 1.632 \quad (6.6a)$$

and

$$\tilde{u}^*(d=3, n=1) = 1.597. \quad (6.6b)$$

Finally, the resulting approximate values of the M_f were converted into estimates for the exponents by inverting the above equations defining M_f in terms of f . Note that we used the hyperscaling relations with $d = 3$. This is why our zeroth approximations (gathered in the column [0/0]) do not always reproduce the Landau (or $\epsilon = 0$) values 0, 1, 0, $\frac{1}{2}$, $\frac{1}{2}$, 1, 3, 2 and 0, 0, $-\frac{1}{2}$, $\frac{1}{2}$ of the exponents $\eta_{\parallel}^{\text{sp}}, \dots, \delta_{11}^{\text{sp}}$ and η_c^*, \dots, Φ listed in the first columns of Tables I/II and III/IV, respectively.

TABLE I. Surface critical exponents of the special transition involving the RG function η_1^{sp} for the case $n = 0$ and $d = 3$.

	O_1/O_2	O_{1i}/O_{2i}	[0/0]	[1/0]	[0/1]	[2/0]	[0/2]	[1/1]	R	R_i^{-1}	$f(\Delta_1, \nu, \eta)$
η_{\parallel}	-1.6	-2.4	0.00	-0.204	-0.169	-0.079	-0.107	-0.126	-0.134	-0.130	-0.133
Δ_1	-4.8	-2.4	0.75	0.954	1.006	0.911	0.886	0.919	0.921	0.926	0.921
η_{\perp}	-1.4	-1.2	0.00	-0.102	-0.114	-0.027	-0.017	-0.059	-0.063	-0.064	-0.053
β_1	0.0	0.0	0.25	0.250	0.250	0.264	0.264	-	-	-	0.255
γ_{11}	-3.6	-2.1	0.50	0.704	0.756	0.647	0.618	0.660	0.663	0.668	0.666
γ_1	-4.5	-2.1	1.00	1.255	1.342	1.199	1.154	1.209	1.212	1.220	1.207
δ_1	-2.3	-1.6	5.00	6.020	6.281	5.576	5.397	5.711	5.739	5.764	5.734
δ_{11}	-2.4	-1.5	3.00	3.816	4.121	3.481	3.283	3.578	3.599	3.628	3.612

TABLE II. Surface critical exponents of the special transition involving the RG function η_1^{sp} for the case $n = 1$ and $d = 3$.

	O_1/O_2	O_{1i}/O_{2i}	[0/0]	[1/0]	[0/1]	[2/0]	[0/2]	[1/1]	R	R_i^{-1}	$f(\Delta_1, \nu, \eta)$
η_{\parallel}	-2.1	-4.8	0.00	-0.266	-0.210	-0.140	-0.174	-0.181	-0.189	-0.183	-0.165
Δ_1	-12.7	-2.9	0.75	1.016	1.113	0.995	0.961	0.997	0.997	1.006	0.997
η_{\perp}	-1.7	-1.4	0.00	-0.133	-0.154	-0.056	-0.040	-0.084	-0.089	-0.091	-0.067
β_1	0.0	0.0	0.25	0.250	0.250	0.261	0.262	-	-	-	0.263
γ_{11}	-8.2	-2.6	0.50	0.766	0.863	0.734	0.695	0.737	0.739	0.747	0.734
γ_1	-11.0	-2.4	1.00	1.333	1.499	1.302	1.237	1.305	1.306	1.320	1.302
δ_1	-4.4	-2.0	5.00	6.331	6.814	6.028	5.779	6.084	6.101	6.147	5.951
δ_{11}	-4.8	-1.8	3.00	4.065	4.650	3.845	3.553	3.882	3.894	3.947	3.791

TABLE III. Surface critical exponents of the special transition involving the RG function η_c^{sp} for the case $n = 0$ and $d = 3$.

	O_1/O_2	O_{1i}/O_{2i}	[0/0]	[1/0]	[0/1]	[2/0]	[0/2]	[1/1]	R	R_i^{-1}	$f(\alpha_1, \nu, \eta)$
η_c^*	-0.7	-0.9	0.00	-0.362	-0.266	0.183	0.055	-0.144	-0.168	-0.160	-0.119
α_1	-1.1	-1.7	0.50	0.217	0.280	0.467	0.399	0.350	0.336	0.342	0.342
α_{11}	-0.8	-1.1	0.00	-0.362	-0.266	0.109	-0.021	-0.157	-0.180	-0.170	-0.140
Φ	-0.4	-0.4	0.50	0.421	0.427	0.642	0.657	0.479	0.474	0.474	0.518

⁹The $n = 0$ value (6.6a) is given by the negative of the value v_2^* of the fixed point denoted U in Ref. [57].

TABLE IV. Surface critical exponents of the special transition involving the RG function η_c^{sp} for the case $n = 1$ and $d = 3$.

	O_1/O_2	O_{1i}/O_{2i}	$[0/0]$	$[1/0]$	$[0/1]$	$[2/0]$	$[0/2]$	$[1/1]$	R	R_i^{-1}	$f(\alpha_1, \nu, \eta)$
η_c^*	-0.7	-1.1	0.00	-0.472	-0.321	0.168	-0.052	-0.200	-0.230	-0.215	-0.144
α_1	-1.4	-2.9	0.50	0.131	0.230	0.393	0.304	0.284	0.268	0.279	0.279
α_{11}	-0.9	-1.6	0.00	-0.472	-0.321	0.042	-0.153	-0.226	-0.253	-0.237	-0.182
Φ	-0.4	-0.4	0.50	0.397	0.407	0.649	0.661	0.470	0.463	0.463	0.539

The quantities O_1 , O_2 , O_{1i} , and O_{2i} appearing in Tables I–IV are defined through the expansions $M_f = 1 + O_1 + O_2 + \dots = [1 + O_{1i} + O_{2i} + \dots]^{-1}$ of the modified quantities $M_f = f/f_0$ or $M_f = f + 1 - f_0$. Using the latter quantity to generate such truncated expansions in the case $|f_0| < 1$ rather than simply factoring out f_0 yields better behaved ‘inverse expansions’, i.e., series for M_f^{-1} .

The bigger the absolute values of the ratios O_1/O_2 and O_{1i}/O_{2i} are, the better is the quality of the resulting series for M_f and its reciprocal $1/M_f$, respectively. All ratios $O_{1(i)}/O_{2(i)}$ have negative sign or else vanish. Thus all series produced by these expansions are alternating, and hence adapted to the above-mentioned Padé-Borel summation technique. (If a series were not alternating, it would be unsuitable for this method because the $[1/1]$ approximant of its Borel transform would have a pole on the positive real axis, i. e., inside the integration range [22].) The estimates obtained via Padé-Borel resummation of the power series for M_f and $1/M_f$ are listed in Tables I–IV as R and R_i^{-1} , respectively.

In most cases the resulting power series in \tilde{u} have second-order corrections $O_{2(i)}$ whose absolute values are smaller than those of their first-order ones. Thus the sequences of associated partial sums appear to be slowly convergent, to the available low order. Exceptions are some series involving η_c^{sp} , whose behavior is rather bad. In the first group of exponents, related to $\eta_1^{\text{sp}}(u)$ and shown in Tables I and II, the most reliable estimates are obtained from the direct series for the exponent Δ_1 , which appear to exhibit the best convergence properties. These estimates are $\Delta_1 = 0.921$ for $n = 0$ and $\Delta_1 = 0.997$ for $n = 1$. Substituting these along with the standard bulk values [23,3] $\nu(n=0) = 0.588$, $\eta(n=0) = 0.027$, $\nu(n=1) = 0.630$, and $\eta(n=1) = 0.031$ into the scaling laws (6.1a)–(6.1g), we have computed the remaining seven exponents of this group. The resulting values $f(\Delta_1, \nu, \eta)$ are presented in the last columns of Tables I and II. By and large, the agreement with the results obtained from the individual expansions is quite reasonable. The deviations of the values $f(\Delta_1, \nu, \eta)$ from the other resummation estimates might serve as a rough measure of the numerical accuracy achieved here.

The situation is less favorable for the second group of exponents, $\eta_c^* \equiv \eta_c^{\text{sp}}(u^*), \dots, \Phi$, whose estimates are given in Tables III and IV. Their series exhibit poor convergence properties. One should be cautious in relying on estimates derived from individual series expansions of an apparently divergent nature, like in the case of the crossover exponent Φ . In this group the exponent α_1 has the estimates with the least scattering. The best series convergence has α_1^{-1} , and the corresponding Padé-Borel estimates are $\alpha_1 = 0.342$ for $n = 0$ and $\alpha_1 = 0.279$ for $n = 1$. Accepting these together with the bulk values of ν and η given above, the estimates of η_c^* , α_{11} , and Φ listed as $f(\alpha_1, \nu, \eta)$ in the last columns of Tables III and IV were derived via scaling laws.

In order to check the quality of our procedure for estimating the numerical values of critical exponents, we have applied the same kind of analysis to the series expansions to second order of the bulk critical exponents. The results are shown in Table V and compared with the estimates of Ref. [23] (last column). The agreement gives us confidence in our method.

The numerical values of surface critical exponents gathered in Tables I–IV generally are in reasonable agreement both with previous estimates based on the ϵ expansion as well as with those obtained by other means. For comparisons we refer to Section III.8 of Ref. [18], where ϵ expansion estimates and estimates that had been gained by alternative techniques till 1985 are given, and to Table VI for more recent results. Note, however, that our estimates for the crossover exponent Φ are definitely lower than the values $\Phi(n=1) \simeq 0.68$ and $\Phi(n=0) \simeq 0.67$ quoted in Ref. [18]. The latter were obtained by setting $\epsilon = 1$ in the ϵ expansion of Φ to order ϵ^2 . On the other hand, recent Monte Carlo simulations yielded the significantly lower estimates $\Phi(1) = 0.461 \pm 0.015$ [42], $\Phi(0) = 0.530 \pm 0.007$ [39], and $\Phi(0) = 0.496 \pm 0.005$ [43]. Our present results $\Phi(1) \simeq 0.54$ and $\Phi(0) \simeq 0.52$ are fairly close to these values.

To see whether comparatively small estimates for $\Phi(n, d=3)$ can be obtained from the ϵ expansion, we have applied the analogous summation techniques to the series

$$2\Phi = 1 + a_1(n)\epsilon + a_2(n)\epsilon^2, \quad (6.7)$$

whose coefficients are known to be [16,18]

$$a_1(n) = -\frac{n+2}{2(n+8)} = -\begin{cases} \frac{1}{8} = 0.125 & \text{for } n = 0 \\ \frac{1}{6} \simeq 0.167 & \text{for } n = 1 \end{cases} \quad (6.8)$$

TABLE V. Numerical estimates of bulk critical exponents.

	O_1/O_2	O_{1i}/O_{2i}	[0/0]	[1/0]	[0/1]	[2/0]	[0/2]	[1/1]	R	R_{inv}^{-1}	Ref. [23]
$n = 0$											
ν	-7.0	-4.1	0.50	0.602	0.614	0.587	0.583	0.589	0.590	0.591	0.588
γ	-4.9	-2.5	1.00	1.204	1.256	1.162	1.137	1.169	1.172	1.177	1.1615
α	-7.0	6.2	0.50	0.194	0.266	0.238	0.238	0.232	0.230	-	0.236
β	-44.1	-13.6	0.25	0.301	0.304	0.300	0.300	0.300	0.300	0.300	0.302
Δ	-6.0	-2.7	1.25	1.505	1.570	1.462	1.434	1.468	1.470	1.477	1.462
$n = 1$											
ν	-27.7	-5.9	0.50	0.633	0.654	0.628	0.624	0.628	0.629	0.630	0.630
γ	-11.3	-2.8	1.00	1.266	1.363	1.243	1.207	1.244	1.245	1.254	1.241
α	-27.7	2.8	0.50	0.101	0.215	0.115	0.148	0.115	0.114	-	0.110
β	14.5	405.8	0.25	0.317	0.321	0.321	0.321	0.321	-	-	0.325
Δ	-17.5	-3.1	1.25	1.583	1.703	1.564	1.525	1.565	1.565	1.575	1.565
$n = 2$											
ν	21.7	-9.1	0.50	0.656	0.685	0.663	0.661	0.663	-	0.664	0.669
γ	∞	-3.2	1.00	1.312	1.453	1.312	1.273	1.312	-	1.322	1.316
α	21.7	1.9	0.50	0.033	0.181	0.011	0.086	0.010	-	-	-0.007
β	7.2	16.5	0.25	0.328	0.334	0.339	0.340	0.340	-	-	0.3455
Δ	36.1	-3.5	1.25	1.640	1.816	1.650	1.609	1.651	-	1.662	1.661
$n = 3$											
ν	9.1	-15.9	0.50	0.673	0.709	0.692	0.693	0.694	-	0.695	0.705
γ	14.5	-3.6	1.00	1.346	1.528	1.370	1.333	1.371	-	1.382	1.386
α	9.1	1.6	0.50	-0.019	0.159	-0.076	0.042	-0.083	-	-	-0.115
β	5.2	9.5	0.25	0.336	0.345	0.353	0.356	0.357	-	-	0.3645
Δ	10.7	-4.0	1.25	1.682	1.910	1.723	1.686	1.727	-	1.739	1.751

TABLE VI. Monte Carlo estimates for surface critical exponents of the special transition in $d = 3$ dimensions.

$n = 0$			
γ_{11}		0.805(15)	Meirovitch & Livne, 1988 [39]
		0.714(6)	Hegger & Grassberger, 1994 [43]
γ_1		1.304(6)	Meirovitch & Livne, 1988 [39]
		1.230(2)	Hegger & Grassberger, 1994 [43]
Φ		0.530(7)	Meirovitch & Livne, 1988 [39]
		0.496(4)	Hegger & Grassberger, 1994 [43]
$n = 1$			
β_1		0.18(2)	Landau & Binder, 1990 [40]
		0.22	Vendruscolo <i>et al.</i> , 1992 [41]
		0.237(5)	Ruge <i>et al.</i> , 1993 [42]
		0.2375(15)	Ruge & Wagner 1995 [44]
γ_{11}		0.96(9)	Landau & Binder, 1990 [40]
		0.788(1)	Ruge & Wagner 1995 [44]
γ_1		1.41(14)	Landau & Binder, 1990 [40]
		1.328(1)	Ruge & Wagner 1995 [44]
Φ		0.59(4)	Landau & Binder, 1990 [40]
		0.74	Vendruscolo <i>et al.</i> , 1992 [41]
		0.461(15)	Ruge <i>et al.</i> , 1993 [42]

and

$$a_2(n) = \frac{n+2}{4(n+8)^3} [8\pi^2(n+8) - (n^2 + 35n + 156)]$$

$$= \begin{cases} \frac{1}{16}\pi^2 - \frac{39}{256} \simeq 0.4645 & \text{for } n = 0. \\ \frac{2}{27}\pi^2 - \frac{16}{81} \simeq 0.5336 & \text{for } n = 1. \end{cases} \quad (6.9)$$

The results are shown in Table VI. It is reassuring that the estimates obtained via Padé-Borel summation compare reasonably well both with our above ones based on the perturbation series at fixed $d = 3$ as well as with the Monte Carlo results mentioned. That these estimates deviate considerably from the values obtained from the $[2/0]$ approximant (6.7) at $\epsilon = 1$ seems to be due to the unusual largeness of the $\mathcal{O}(\epsilon^2)$ term of Φ . In summary, we conclude that the values of the crossover exponent $\Phi(n, d)$ with $n = 0, 1$ and $d = 3$ are indeed significantly smaller than previously thought, being close to 0.5.

TABLE VII. Estimates for $\Phi(n, d=3)$ based on the ϵ expansion.

n	O_1/O_2	O_{1i}/O_{2i}	[0/0]	[1/0]	[0/1]	[2/0]	[0/2]	[1/1]	R	R_i^{-1}
0	-0.27	-0.28	0.5	0.438	0.444	0.670	0.740	0.487	0.482	0.483
1	-0.31	-0.33	0.5	0.417	0.429	0.683	0.757	0.480	0.474	0.475

An interesting aspect of the above results is worth mentioning: We may be quite confident that the inequality

$$\alpha_{11}^{\text{sp}} < 0 \quad (6.10)$$

is satisfied for $d = 3$ and $n = 1$. For one thing, our best numerical estimate based on the massive RG approach at fixed $d = 3$ is $\alpha_{11}^{\text{sp}}(n = 1, 3) \simeq -0.18$. Second, the scaling relation (6.3b) can be rewritten at $d = 3$ as

$$\alpha_{11}^{\text{sp}}(n, 3)(n, d=3) = -2(\nu - \Phi). \quad (6.11)$$

In view of the various estimates given above it seems rather unlikely that $\Phi(1, 3)$ will be larger than $\nu(1, 3) \simeq 0.630$, so that (6.10) should be valid at $d = 3$ and $n = 1$, a conclusion which may also be reached for $n = 0$.

This has important consequences. As has been shown in Ref. [58], (6.10) plays the role of an *irrelevance criterion* for *weak, short-range correlated randomness* that couples to the *surface energy density* (and is restricted to the surface). If it is satisfied, the fixed point describing the special transition of the pure model is *stable* with respect to this kind of randomness, so that such random “surface-enhancement disorder” should be *irrelevant* at the special transition. According to our numerical estimates, this irrelevance should indeed apply. It has been verified by Monte Carlo simulations recently [59].

VII. ORDINARY TRANSITION

In our analysis of the asymptotic critical behavior at the special transition it turned out to be advantageous to set the bare and renormalized surface enhancements to their respective critical values $c_0 = c_0^{\text{sp}}$ and $c = 0$. The benefit was that we did not have to deal with renormalization functions depending on *two* mass parameters m and c , a fact which facilitated the computation of the required Feynman graphs considerably.

In the case of the ordinary transition we must study the limit $c/m \rightarrow \infty$. For the sake of achieving a similar simplification, it would be desirable to set $c = \infty$ (or $c_0 = \infty$) from the outset. In doing so one is faced with a known difficulty: Studying the functions $G^{(N,M)}$ with $c_0 = \infty$ does not easily give access to surface critical exponents via the RG equations of their renormalized analogs because these bare functions as well as the renormalized ones with $c = \infty$ satisfy *Dirichlet boundary conditions*. Fortunately it is known from previous studies based on alternative RG approaches [14,15,18,60] how this problem can be overcome: one must study the functions

$$\mathcal{G}^{(N,M)}(\mathbf{x}_1, \dots, \mathbf{r}_M) \equiv \left\langle \left[\prod_{j=1}^N \phi^{a_j}(\mathbf{x}_j) \right] \left[\prod_{k=1}^M \partial_n \phi^{b_k}(\mathbf{r}_k) \right] \right\rangle^{\text{cum}}, \quad (7.1)$$

where ∂_n means the derivative along the inner normal. The functions $\mathcal{G}^{(N,M)}$ with $M > 0$ do not vanish for $c_0 = \infty$, and the scaling dimension of $\partial_n \phi$ yields $\eta_{\parallel}^{\text{ord}}$, the sole missing surface exponent.¹⁰

That the relevant information can be obtained from these functions can be seen either by expanding the bare cumulants $G^{(N,M)}$ in powers of c_0^{-1} or by noting that because of the Dirichlet boundary condition $\partial_n \phi$ is the leading operator appearing in the boundary operator expansion [15,18] of ϕ .

A. General considerations and the limit $c/m \rightarrow \infty$

Let us denote the functions $\mathcal{G}^{(N,M)}$ with $c_0 = \infty$ as $\mathcal{G}_{\infty}^{(N,M)}$. Although we shall not present a complete analysis of the c -dependent normalization conditions of Sec. III B and of the crossover from special to ordinary surface critical behavior here, we will at least verify that this renormalization procedure is consistent with the one based on the $\mathcal{G}_{\infty}^{(N,M)}$, a scheme whose results were briefly described in Ref. [38] and which will be exploited below.

We start by performing the mass renormalization as described in Appendix A 1, and introduce $\hat{\sigma}(p; m, c_0)$, the analog of $\hat{\sigma}_0(p)$, via

$$\hat{G}^{(0,2)}[p; m_0(m), u_0, c_0] = [\kappa + c_0 - \hat{\sigma}(p; m, c_0)]^{-1}. \quad (7.2)$$

Its expansion to order u_0^2 is given in (A16) of Appendix A 1.

Assuming that the renormalized surface enhancement c has an arbitrary value $0 \leq c < \infty$, we imagine that the surface-enhancement renormalization has been carried out in the way explained in Appendix A 2. Substituting the resulting form (A19) of $[\hat{G}^{(0,2)}(p)]^{-1}$ into (5.2a) yields

$$[Z_1(u, c/m)Z_{\phi}(u)]^{-1} - 1 = -\lim_{p \rightarrow 0} \frac{m}{p} \frac{\partial}{\partial p} [\hat{\sigma}(p; m, c + \delta c) - \hat{\sigma}(0; m, c + \delta c)]. \quad (7.3)$$

We wish to study what happens to the perturbation expansion in u of the right-hand side of (7.3) in the limit $c/m \rightarrow \infty$. To this end, we set $m = 1$ and let $c \rightarrow \infty$. Then the free propagator — namely (2.6), with c_0 and κ_0 replaced by c and κ , respectively — goes over into the Dirichlet propagator (A3). Further, the perturbative corrections caused by the shift δc to the term inside the square brackets of (7.3) vanish as $c \rightarrow \infty$.¹¹ Hence we have

$$\lim_{c \rightarrow \infty} [\hat{\sigma}(p; m, c + \delta c) - \hat{\sigma}(0; m, c + \delta c)] = \hat{\sigma}^{(D)}(p; m) - \hat{\sigma}^{(D)}(0; m) \quad (7.4)$$

with $\hat{\sigma}^{(D)}(p; m) = \hat{\sigma}(p; m, \infty)$. As we have seen, the graphs of $\hat{\sigma}^{(D)}(p; m)$ are obtained from those of $\hat{\sigma}(p; m, c)$ by associating with all full lines the Dirichlet propagator \hat{G}_D rather than the c -dependent one (2.6), and with all full lines labeled “s” (cf. Appendix A 1) its surface part, given by (A12) with $c_0 = \infty$. Note that these graphs are not in general uv finite at $d = 3$. But subtraction of their values at $p = 0$, which is provided by the last term in (7.4), is sufficient to make them so. In other words, in the limit $c \rightarrow \infty$, surface-enhancement renormalization reduces to an additive renormalization.

To see how this relates to our approach based on the $c_0 = \infty$ functions $\mathcal{G}_{\infty}^{(N,M)}$, we return to the representation (5.5) of $\hat{\sigma}_0$ in terms of the self-energy $\hat{\Sigma}$. Since the denominator of the fraction in (5.5) becomes one for $c_0 = \infty$, we have $\hat{\sigma}^{(D)} = \hat{g}^T \hat{T}[G_D] \hat{g}$, where $T[G]$ is the T-matrix introduced in (5.4). Now the reduced propagator (5.6) can be written as

$$\hat{g}(p; z') = e^{-\kappa z'} = \frac{\partial}{\partial z} \hat{G}_D(\mathbf{p}; z, z') \Big|_{z=0}. \quad (7.5)$$

Thus we get

$$\hat{\mathcal{G}}_{\infty}^{(0,2)}[p; m_0(m)] = -\kappa + \hat{\sigma}^{(D)}(p; m), \quad (7.6)$$

¹⁰Since the scaling dimension $\Delta[\varepsilon_1]$ of the surface energy density ε_1 at the ordinary transition is exactly given by $\Delta[\varepsilon_1] = d$, the analogs of (6.3a) and (6.3b) read $\alpha_1^{\text{ord}} = \alpha - 1$ and $\alpha_{11}^{\text{ord}} = \alpha - 2 - \nu$, respectively [60,15]. The other surface exponents are given by the scaling relations (6.1).

¹¹A simple way to see this is to note that such corrections involve free propagators with points on the surface. Dimensional arguments lead to the same conclusion.

where it should be remembered [17,18,60] that $\partial_z \partial_{z'} \hat{G}_D(p; z, z')$ has a contribution of the form $[-\delta(z - z')]$; we have dropped the implied singularity $[-\delta(0)]$ in the zero-loop term $(-\kappa)$, interpreting $\partial_n \hat{G}_D \overleftarrow{\partial}_n$ as the limit of $\partial_z \partial_{z'} \hat{G}_D(p; z, z')$ as $z, z' \rightarrow 0$ with $z \neq z'$. Combining these findings with (7.3) and (7.4) yields

$$[Z_1(u, \infty) Z_\phi(u)]^{-1} = - \lim_{p \rightarrow 0} \frac{m}{p} \frac{\partial}{\partial p} \left[\hat{\mathcal{G}}_\infty^{(0,2)}(p) - \hat{\mathcal{G}}_\infty^{(0,2)}(0) \right]. \quad (7.7)$$

Next, let us recapitulate our renormalization scheme for the $\mathcal{G}_\infty^{(N,M)}$ [38]. Aside from the previous bulk renormalization functions, it involves a renormalization factor $Z_{1,\infty}(u)$, which enters the definition of the renormalized surface operator:

$$(\partial_n \phi)_{\text{ren}} = [Z_{1,\infty} Z_\phi]^{-1/2} \partial_n \phi, \quad (7.8)$$

and of the renormalized functions:

$$\hat{\mathcal{G}}_{\infty, \text{ren}}^{(N,M)}(\{\mathbf{p}\}; \{z_j\}; m, u) = Z_\phi^{-(N+M)/2} Z_{1,\infty}^{-M/2} \left[\hat{\mathcal{G}}_\infty^{(N,M)}(\{\mathbf{p}\}; \{z_j\}) - \delta_{N,0}^{M,2} \hat{\mathcal{G}}_\infty^{(0,2)}(0) \right]. \quad (7.9)$$

One evident normalization condition is

$$\hat{\mathcal{G}}_{\infty, \text{ren}}^{(0,2)}(0; m, u) = 0. \quad (7.10a)$$

The other,

$$\frac{\partial}{\partial p^2} \hat{\mathcal{G}}_{\infty, \text{ren}}^{(0,2)}(p; m, u) \Big|_{p=0} = -\frac{1}{2m}, \quad (7.10b)$$

(suggested by the corresponding zero-loop result) serves to fix $Z_{1,\infty}$. In conjunction with (7.9) it implies the relation:

$$Z_{1,\infty}(u) Z_\phi(u) = - \lim_{p \rightarrow 0} \frac{m}{p} \frac{\partial}{\partial p} \left[\hat{\mathcal{G}}_\infty^{(0,2)}(p) - \hat{\mathcal{G}}_\infty^{(0,2)}(0) \right], \quad (7.11)$$

whose comparison with (7.7) reveals that

$$\left[Z_1(u, \infty) Z_\phi(u) \right]^{-1} = \lim_{c/m \rightarrow \infty} \left[Z_1(u, c/m) Z_\phi(u) \right]^{-1} = Z_{1,\infty}(u) Z_\phi(u) \quad (7.12)$$

to any order of perturbation theory.

We introduce the analog of the exponent function η_1^{sp} by

$$\eta_{1,\infty}(u) \equiv \tilde{\eta}_{1,\infty}(\tilde{u}) \equiv m \frac{\partial}{\partial m} \Big|_0 \ln Z_{1,\infty}(u) = \beta(u) \frac{\partial \ln Z_{1,\infty}(u)}{\partial u}, \quad (7.13)$$

where \tilde{u} is the rescaled coupling constant of (5.8). The fixed-point value of this function, $\eta_{1,\infty}(u^*)$, is related to $\eta_{\parallel}^{\text{ord}}$ via [38] (cf. Ref. [18])

$$\eta_{\parallel}^{\text{ord}} = 2 + \eta_1^{\text{ord}}(u^*) + \eta_\phi(u^*), \quad (7.14)$$

as we shall verify below. Reasoning in a standard fashion, we find that

$$Z_{1,\infty} \sim (u - u^*)^{\eta_{1,\infty}(u^*)/\omega} \sim m^{\eta_{1,\infty}(u^*)} \quad (7.15)$$

as $m \rightarrow 0$ (or $u \rightarrow u^*$), with fixed bare interaction constant u_0 (and $c_0 = \infty$).

The renormalized functions $G_{\infty, \text{ren}}^{(N,M)}$ satisfy the analog of the CS equation (4.3a):

$$\left[m \frac{\partial}{\partial m} + \beta(u) \frac{\partial}{\partial u} + \frac{N+M}{2} \eta_\phi(u) + \frac{M}{2} \eta_{1,\infty}(u) \right] G_{\infty, \text{ren}}^{(N,M)}(; m, u) = \Delta G_{\infty, \text{ren}}, \quad (7.16)$$

in which the inhomogeneous term $\Delta G_{\infty, \text{ren}}$ is defined just as ΔG_{ren} in (4.3b), but with $G_{\text{ren}, \text{sp}}^{(N,M;1,0)}$ replaced by $G_{\infty, \text{ren}}^{(N,M;1,0)}$, the corresponding cumulant with an insertion of $\frac{1}{2} \int_V \phi^2$. Neglecting $\Delta G_{\infty, \text{ren}}$, we can exploit in the usual

The required u_0^2 term is easily calculated (see Appendix B). One finds

$$Z_{1,\infty} Z_\phi = 1 + \frac{n+2}{12} \frac{u_0}{8\pi m} + \frac{n+2}{3} \left(\frac{u_0}{8\pi m} \right)^2 C + \mathcal{O}(u_0^3) \quad (7.25a)$$

with

$$C = \frac{107}{162} - \frac{7}{3} \ln \frac{4}{3} - 0.094299 = -0.105063. \quad (7.25b)$$

Upon expressing u_0 in terms of the rescaled renormalized coupling constant $\tilde{u} = u(n+8)/48m\pi$ [cf. (5.8)], the result becomes

$$Z_{1,\infty}(u) Z_\phi(u) = 1 + \frac{n+2}{2(n+8)} \tilde{u} + \frac{12(n+2)}{(n+8)^2} \left(C + \frac{n+8}{24} \right) \tilde{u}^2 + \mathcal{O}(u^3). \quad (7.26)$$

From it the exponent function appearing on the right-hand side of (7.14) can be deduced in a straightforward fashion. One obtains

$$\eta_{\parallel}^{\text{ord}}(u) = \tilde{\eta}_{\parallel}^{\text{ord}}(\tilde{u}) = 2 - \frac{n+2}{2(n+8)} \tilde{u} - \frac{24(n+2)}{(n+8)^2} \left(C + \frac{n+14}{96} \right) \tilde{u}^2 + \mathcal{O}(u^3). \quad (7.27)$$

The corresponding series expansions of the surface exponents Δ_1^{ord} , $\eta_{\perp}^{\text{ord}}$, β_1^{ord} , γ_{11}^{ord} , γ_1^{ord} , δ_1^{ord} , and δ_{11}^{ord} follow again by substituting (7.27) together with the expansions (6.2) of ν and η into the scaling-law expressions (6.1).

C. Numerical estimates for the surface critical exponents of the ordinary transition

Following the strategy described in Sec. VI, one can analyze the above power series for the critical exponents of the ordinary transition and extract numerical estimates. The results are shown in Tables VIII-XI, where the entries have the same meaning as in Tables I-II (Sec. VI). As before, the fixed-point values $u^*(n)$ of Refs. [21] and [57], obtained by Padé-Borel resummation of the two-loop result for the β function, were used.

TABLE VIII. Surface critical exponents of the ordinary transition for $d = 3$ and $n = 0$. As fixed-point value we used $\tilde{u}^* = 1.632$.

	O_1/O_2	O_{1i}/O_{2i}	[0/0]	[1/0]	[0/1]	[2/0]	[0/2]	[1/1]	$f(\eta_{\parallel}, \nu, \eta)$
η_{\parallel}	2.5	2.0	2.00	1.796	1.815	1.715	1.734	1.660	1.660
Δ_1	4.4	7.8	0.25	0.352	0.364	0.375	0.380	0.382	0.394
η_{\perp}	3.6	2.6	1.00	0.898	0.907	0.870	0.877	0.859	0.843
β_1	-1.9	-1.6	0.75	0.852	0.864	0.799	0.790	0.817	0.782
γ_{11}	0.0	0.0	-0.50	-0.500	-0.500	-0.424	-0.434	-	-0.388
γ_1	15.4	-11.4	0.50	0.653	0.681	0.663	0.662	0.664	0.680
δ_1	2.5	3.1	1.67	1.780	1.788	1.825	1.832	1.854	1.870
δ_{11}	2.1	2.7	0.33	0.424	0.433	0.466	0.476	0.504	0.504

TABLE IX. Surface critical exponents of the ordinary transition for $d = 3$ and $n = 1$. As fixed-point value we used $\tilde{u}^* = 1.597$.

	O_1/O_2	O_{1i}/O_{2i}	[0/0]	[1/0]	[0/1]	[2/0]	[0/2]	[1/1]	$f(\eta_{\parallel}, \nu, \eta)$
η_{\parallel}	2.3	1.8	2.00	1.734	1.765	1.618	1.655	1.528	1.528
Δ_1	3.0	5.0	0.25	0.383	0.404	0.427	0.440	0.450	0.464
η_{\perp}	3.0	2.2	1.00	0.867	0.883	0.823	0.837	0.801	0.779
β_1	-2.5	-1.9	0.75	0.883	0.904	0.829	0.815	0.845	0.796
γ_{11}	0.0	0.0	-0.50	-0.500	-0.500	-0.402	-0.418	-	-0.333
γ_1	5.7	-40.4	0.50	0.700	0.749	0.735	0.742	0.742	0.769
δ_1	2.2	2.7	1.67	1.815	1.829	1.883	1.898	1.941	1.966
δ_{11}	1.9	2.5	0.33	0.452	0.468	0.514	0.533	0.582	0.582

TABLE X. Surface critical exponents of the ordinary transition for $d = 3$ and $n = 2$. As fixed-point value we used $\tilde{u}^* = 1.558$.

	O_1/O_2	O_{1i}/O_{2i}	[0/0]	[1/0]	[0/1]	[2/0]	[0/2]	[1/1]	$f(\eta_{ }, \nu, \eta)$
$\eta_{ }$	2.2	1.6	2.00	1.688	1.730	1.545	1.598	1.422	1.422
Δ_1	2.4	3.9	0.25	0.406	0.435	0.470	0.493	0.514	0.528
η_{\perp}	2.7	1.9	1.00	0.844	0.865	0.787	0.808	0.753	0.727
β_1	-3.2	-2.1	0.75	0.906	0.935	0.856	0.840	0.868	0.810
γ_{11}	0.0	0.0	-0.50	-0.500	-0.500	-0.387	-0.408	-	-0.282
γ_1	3.9	42.1	0.50	0.734	0.805	0.794	0.814	0.815	0.851
δ_1	2.0	2.5	1.67	1.840	1.860	1.928	1.952	2.019	2.051
δ_{11}	1.8	2.3	0.33	0.472	0.494	0.550	0.579	0.651	0.652

 TABLE XI. Surface critical exponents of the ordinary transition for $d = 3$ and $n = 3$. As fixed-point value we used $\tilde{u}^* = 1.521$.

	O_1/O_2	O_{1i}/O_{2i}	[0/0]	[1/0]	[0/1]	[2/0]	[0/2]	[1/1]	$f(\eta_{ }, \nu, \eta)$
$\eta_{ }$	2.1	1.5	2.00	1.654	1.705	1.489	1.556	1.338	1.338
Δ_1	2.1	3.4	0.25	0.423	0.459	0.504	0.538	0.574	0.586
η_{\perp}	2.5	1.8	1.00	0.827	0.853	0.759	0.787	0.714	0.685
β_1	-4.1	-2.4	0.75	0.923	0.959	0.880	0.862	0.889	0.824
γ_{11}	0.0	0.0	-0.50	-0.500	-0.500	-0.377	-0.401	-	-0.238
γ_1	3.1	16.3	0.50	0.759	0.850	0.842	0.880	0.882	0.927
δ_1	1.8	2.3	1.67	1.859	1.884	1.963	1.995	2.088	2.124
δ_{11}	1.7	2.3	0.33	0.487	0.515	0.578	0.617	0.711	0.711

For most of the obtained truncated series expansions, the coefficients do not alter in sign, and the truncated series of their reciprocal (i.e., their ‘inverse series’) display a similar behavior. Of this kind are the series for $\eta_{||}^{\text{ord}}$, Δ_1^{ord} , $\eta_{\perp}^{\text{ord}}$, δ_1^{ord} , and δ_{11}^{ord} with $n = 0, \dots, 3$, and for γ_1^{ord} with $n = 2$ and 3. Let $s_{[p/q]}$, with $p + q \leq 2$, be the values resulting from Padé approximants of type $[p/q]$ (and listed in the columns marked $[p/q]$), and let $s_p \equiv s_{[p/0]}$. Looking at Tables VIII–XI one realizes that the sequences of values $s_{[p/q]}$ associated with each one of these critical indices have the following feature: The values move away from s_0 such that the second-order approximants $[p/(2-p)]$ give values farther away from s_0 than the first-order ones $[p/(1-p)]$ and that furthermore $s_{[1/1]}$ is the most distant one. In other words, either they increase according to

$$s_0 < s_1 < s_2 < s_{[1/1]} \quad \text{and} \quad s_0 < s_{[0/1]} < s_{[0/2]} < s_{[1/1]} \quad (7.28)$$

or else they decrease in the corresponding fashion. In most cases even the stronger chain of inequalities

$$s_0 < \min \{s_1, s_{[0/1]}\} < \max \{s_1, s_{[0/1]}\} < \min \{s_2, s_{[0/2]}\} < \max \{s_2, s_{[0/2]}\} < s_{[1/1]} \quad (7.29)$$

or its decreasing analog applies.

The value $s_{[1/1]}$ always comes last in these sequences. Using it to extrapolate the series amounts to anticipating that the next (thus far unknown) terms of the power series expansion in \tilde{u} have coefficients of the same sign. This assumption might well be true for some of the series (an example of this kind is the bulk exponent η), and in view of the just mentioned feature of the $s_{[p/q]}$ with $p + q \leq 2$ it seems legitimate to us to accept it. Accordingly we consider $s_{[1/1]}$ to be the best among all those estimates $s_{[p/q]}$ with $p + q \leq 2$ for a given exponent that we obtained from its individual series expansion.

For γ_1^{ord} with $n = 0$ and 1, only the first chain of inequalities of (7.28) holds. Its inverse series has first-order and second-order corrections of different signs, and hence may be treated by the Padé-Borel method. The resulting resummation values (the analog of the ones denoted R_i^{-1} in Tables I–IV) agree with $s_{[1/1]}$ up to three decimals.

In the case of β_1^{ord} (with $n = 0, 1, 2, 3$) both the direct and the inverse series are alternating. The results of our resummations differ from the values of the $[1/1]$ approximants only in the third decimal. (Therefore we have not listed them separately.) The series for γ_{11}^{ord} have zero first-order corrections and hence are not well adapted for estimating this critical exponent.

In order to gain further improved estimates, we follow a similar strategy as we did in Sec. VI when estimating the critical exponents of the special transition: we try to exploit the above results in conjunction with the available high-precision estimates for the bulk exponents ν and η . To this end we substitute our $[1/1]$ values for $\eta_{||}^{\text{ord}}$, together with the estimates taken from Ref. [23], $\nu = 0.588$, $\eta = 0.027$ (for $n = 0$), $\nu = 0.630$, $\eta = 0.031$ (for $n = 1$), $\nu = 0.669$,

$\eta = 0.033$ (for $n = 2$), and $\nu = 0.705$, $\eta = 0.033$ (for $n = 3$), into the scaling-law expressions (6.1). The results are given as $f(\eta_{\parallel}, \nu, \eta)$ in the last row of Tables VIII-XI. As one sees, in those cases in which the Padé values $s_{[p/q]}$ move away from s_0 in a given direction such that either (7.28) — or even (7.29) — or else their corresponding decreasing analogs hold, the estimates $f(\eta_{\parallel}, \nu, \eta)$ turn out to be displaced even further in the same direction.

We consider our estimates $f(\eta_{\parallel}, \nu, \eta)$ as the best we could attain from the available knowledge on the series expansions, within the present approximation scheme. In some cases they differ significantly from the zeroth-order values s_0 we started from. Like in the case of the special transition, our best estimates agree reasonably well both with the earlier ones based on the ϵ expansion [18,61] as well as with more recent computer-simulation results [39,43,59,62–65]. The latter are gathered in Table XII. For references to earlier numerical estimates and their comparison with ϵ -expansion results, the reader may consult Ref. [18].

TABLE XII. Monte Carlo estimates for the surface critical exponents of the ordinary transition in $d = 3$ dimensions.

$n = 0$			
γ_{11}	−0.38(2)		Meirovitch & Livne, 1988 [39]
	−0.353(17)		De’Bell <i>et al.</i> , 1990 [62]
	−0.383(5)		Hegger & Grassberger, 1994 [43]
γ_1	+0.718(8)		De’Bell & Lookman, 1985 [63]
	+0.687(5)		Meirovitch & Livne, 1988 [39]
	+0.694(4)		De’Bell <i>et al.</i> , 1990 [62]
	+0.679(2)		Hegger & Grassberger, 1994 [43]
$n = 1$			
β_1	+0.79(2)		Kikuchi & Okabe, 1985 [64]
	+0.78(2)		Landau & Binder, 1990 [40]
	+0.75(2)		Ruge <i>et al.</i> , 1993 [42]
	+0.807(4)		Ruge & Wagner, 1995 [44]
	+0.80 ± 0.01		Pleimling & Selke, 1998 [59]
γ_1	+0.78(6)		Landau & Binder, 1990 [40]
	+0.760(4)		Ruge & Wagner, 1995 [44]
	+0.78 ± 0.05		Pleimling & Selke, 1998 [59]
γ_{11}	−0.25 ± 0.1		Pleimling & Selke, 1998 [59]
δ_1	+2.00(8)		Kikuchi & Okabe, 1985 [64]
$n = 2$			
β_1	+0.84		Landau <i>et al.</i> , 1989 [65]
γ_1	$\simeq \frac{2}{3}$		Landau <i>et al.</i> , 1989 [65]

Specifically, our estimates $\gamma_{11}^{\text{ord}}(n=0) \simeq -0.388$ and $\gamma_1^{\text{ord}}(n=0) \simeq 0.680$ for the polymer universality class ($n = 0$) are in excellent agreement with the recent (apparently very precise) Monte Carlo estimates $\gamma_{11}^{\text{ord}}(n=0) = -0.383(5)$ and $\gamma_1^{\text{ord}}(n=0) = 0.679(2)$ by Hegger and Grassberger [43]. Likewise for the Ising universality class, our numerical values $\beta_1^{\text{ord}}(n=1) \simeq 0.80$ and $\gamma_1^{\text{ord}}(n=1) \simeq 0.77$ are very close to the Monte Carlo estimates $\beta_1^{\text{ord}}(n=1) = 0.807(4)$ and $\gamma_1^{\text{ord}}(n=1) = 0.760(4)$ of Ruge *et al.* [44]. Landau and Binder’s earlier Monte Carlo estimates [40] $\beta_1^{\text{ord}}(n=1) \simeq 0.78$ and $\gamma_1^{\text{ord}}(n=1) = 0.78(6)$ are slightly smaller and larger, respectively. The more recent ones by Pleimling and Selke [59] coincide within their error bars with those of Ref. [44] and our best estimate.

There also exist some experimental results¹² with which these theoretical Ising values can be compared. Sigl and Fenzl [67] were able to extract the value $\beta_1 = 0.83 \pm 0.05$ from capillary-rise experiments on the transition from partial to complete wetting in critical mixtures of lutidine and water with different amounts of dissolved potassium chloride. Using the technique of x-ray scattering at grazing incidence [68,69,66,70], Mailänder *et al.* [71] investigated the surface critical behavior of a FeAl alloy at its *B2-DO3* disorder-order transition [72–74]. The values $\eta_{\parallel} = 1.52 \pm 0.04$, $\beta_1 = 0.75 \pm 0.06$, and $\gamma_{11} = -0.33 \pm 0.06$ they found are consistent with our estimates¹³ $\eta_{\parallel}^{\text{ord}}(n=1) \simeq 1.53$, $\beta_1^{\text{ord}}(n=1) \simeq 0.80$, and $\gamma_{11}^{\text{ord}}(n=1) \simeq -0.33$ (taken from the last column of Table IX).

¹²For background and a review of experimental work on surface critical behavior, see Ref. [66].

¹³The case of the *B2-DO3* transition is more complicated than that of the *A2-B2* transition, for the *DO3* structure involves four sublattices and hence a larger number of composition variables [72]. Nevertheless the *B2-DO3* transition is expected to belong to the Ising universality class [73,74]; see the note added in proof in Ref. [19].

An x-ray scattering experiment has also been performed on the A2-B2 disorder-order transition in a semi-infinite FeCo alloy that is bounded by a (001) surface [75]. This yielded $\beta_1 = 0.79 \pm 0.10$, in conformity with the above theoretical values for $\beta_1^{\text{ord}}(n=1)$. Yet it should be noted that the chosen (001) surface *breaks* the symmetry of interchanging the two sublattices [76–78]. Therefore the Hamiltonian one encounters in a coarse-grained continuum description of the large-scale physics is *not* invariant under a sign change $\phi \rightarrow -\phi$ of the order parameter and will generically have surface contributions involving *odd* powers of ϕ and its derivatives [79,18]. In particular, surface contributions *linear* in ϕ , i.e., a *surface ordering field* $g_1 \neq 0$, normally should be present, and since g_1 is a relevant scaling field, the asymptotic critical behavior must be characteristic of the *normal*¹⁴ [80,19] rather than the ordinary transition [77,78].

In their experiment, Krimmel *et al.* [75] actually found evidence of the presence of such a surface ordering field g_1 . On the other hand, they did not observe the crossover to the normal surface transition. The reason seems to be that g_1 is rather small. In order to see clear manifestations of this crossover or even verify the true asymptotic behavior, one must therefore resolve a temperature regime fairly close to T_c . The one studied in the experiment was apparently not close enough, a possibility which has already been suggested by the experimentalists themselves [75]. A recent reanalysis [81] of their data indicates that these are even better consistent with the behavior one should expect near T_c when the scaling variable $g_1|\tau|^{-\Delta_1^{\text{ord}}}$ is still small (so that the crossover to the normal surface transition has not yet set in) than the original analysis by Krimmel *et al.* revealed.

The experiments [71] on the B2-DO3 transition of FeAl also require a comment. Just as in the measurements on FeCo [75], a small amount of long-range order near the surface was found to persist at and above T_c . It is tempting to attribute this again to the presence of a surface ordering field g_1 (cf. Ref. [66]). However, the orientation of the surface plane of the FeAl crystal investigated in Ref. [71] was symmetry *preserving* in the sense of Refs. [76] and [78], so surface contributions breaking the $\phi \rightarrow -\phi$ symmetry of the Hamiltonian should not occur. Thus, if the explanation of the experimental findings must indeed be sought in the presence of a surface ordering field, then the question of its origin arises.¹⁵ It appears that further theoretical and experimental work is required to clarify this issue.

X-ray scattering experiments have also been performed on a NH₄Br single crystal [82]. The authors argue that the critical fluctuations at the observed order-disorder transition should be described by the three-dimensional Ising model, but also point out that the transition is coupled to a first-order displacive transition. The effective exponents they measured, $\eta_{\parallel} = 1.3 \pm 0.15$ and $\beta_1 = 0.8 \pm 0.1$, are compatible with the theoretical predictions for the $n=1$ ordinary transition. In view of the coupling to the displacive transition it is however not clear to us how serious such a comparison can be taken.

Our estimates for $n=2$ and 3, given in Tables X and XI, also conform nicely with the previous ϵ -expansion estimates gathered in Table VI (p. 186) of Ref. [18], from which we quote the value $\eta_{\parallel}^{\text{ord}}(n=2) \simeq 1.38$ as an example (to be compared with our present best estimate $\simeq 1.42$). For $n=2$, there exist some recent Monte-Carlo results by Landau *et al.* [65], as mentioned in Table XII. For a comparison with series-expansion estimates for the cases $n=2$ and 3, we refer to Table VII of Ref. [18] and the original work [83].

Our values $\eta_{\parallel}^{\text{ord}}(n=3) \simeq 1.34$ and $\beta_1^{\text{ord}}(n=3) \simeq 0.82$ are fairly close to the estimates $\eta_{\parallel}^{\text{ord}}(n=3) \simeq 1.29 \pm 0.02$ and $\beta_1^{\text{ord}}(n=3) \simeq 0.84 \pm 0.01$ Diehl and Nüsser [61] obtained from Padé approximants that exploited the results of both the ϵ expansion and the $d-2$ expansion to second order. We are not aware of any recent Monte-Carlo predictions for surface critical exponents of the $n=3$ ordinary transition. On the experimental side, there is the result $\beta_1 = 0.825^{+0.025}_{-0.040}$ Alvarado *et al.* [84] found for a Ni(100) surface using spin-polarized low-energy electron diffraction.

VIII. CONCLUDING REMARKS

In this work we have extended the massive field-theory approach for studying critical behavior in a fixed space dimension below the upper critical dimension to systems with surfaces. We have carried out two-loop calculations for the ordinary and special surface transitions in $d=3$ bulk dimensions and performed a Padé-Borel analysis of the resulting series for the respective surface critical exponents. The behavior of the truncated series we have obtained

¹⁴A justification of the name “normal surface transition” may be found, for example, in Refs. [80] and [19].

¹⁵Any real surface will, of course, not be ideally planar. Hence the symmetry invoked in proving the absence of symmetry-breaking terms in the Hamiltonian [78] will not be strictly realized. Nevertheless, one would not expect such unavoidable imperfections to manifest themselves through symmetry-breaking contributions proportional to the surface area, unless the crystal was not carefully prepared and its surface not well-defined.

and analyzed, though less good-natured for some than for other exponents, is in general very similar to what one finds for those of bulk exponents at the same two-loop order of truncation. We take this as a clear indication of the potential power of the approach: when pushed to an order of perturbation theory that is comparable to what has been achieved for the bulk exponents [3,21–23,85] and investigated by the same sophisticated techniques based on Borel summation and large-order analysis, it should yield similarly precise numerical estimates.

One motivation for the present study was to see whether the field-theory results might be reconciled with the small values of $\simeq 0.5$ found in recent Monte Carlo simulations [42,43] for the crossover exponents $\Phi(d=3, n)$ with $n=0$ and $n=1$. Our present best estimates $\Phi(3, n=0) \simeq 0.52$ and $\Phi(3, n=1) \simeq 0.54$ (cf. Tables III and IV) are indeed much lower than the original ones based on the ϵ expansion (which were $\simeq 0.67$ and $\simeq 0.68$, respectively [16,18]), and as we have seen, a Padé-Borel analysis of the ϵ expansion to order ϵ^2 yields comparatively low $d=3$ estimates. That the original ϵ -expansion estimates for Φ were $\simeq 20\%$ greater than our present ones seems to be due to the unusual largeness of its $\mathcal{O}(\epsilon^2)$ terms, which entails that the value of the truncated power series at $\epsilon=1$ gives a rather poor approximation for $\Phi(d=3)$. This problem exist, of course, also for the other surface exponents that derive from the same RG function η_c as Φ (such as α_1^{sp} , cf. Tables III and IV). For the remaining surface exponents of both transitions, the $\mathcal{O}(\epsilon^2)$ terms are much smaller, so the values of the truncated series at $d=3$ turn out to be much closer to our best estimates.

In those cases in which there is little difference between the ϵ -expansion values given in Ref. [18] and our best estimates here, one may say that these field-theory values have been put on a more reliable basis by our present analysis because of our use of better extrapolation procedures based on Padé-Borel summation techniques.

To give error bars for our estimates of surface critical exponent is a rather delicate matter. If we took as a measure of uncertainty for the value of any given one of them the spread of values of the various extrapolations of the $\mathcal{O}(u^2)$ series expansion, then a reasonable guess might be a typical accuracy of a few, say, 5%. What appears to be needed most for an improvement of the accuracy and more reliable error bars is the computation of the series coefficients of the surface exponents to a higher order in perturbation theory.

There is an additional problem one is faced with in massive field-theory approaches to systems with boundaries that should be mentioned: the appearance of further mass scales such as the renormalized surface enhancement c . Having to deal with more than one mass parameter, namely with m and the ratio c/m , makes calculations rather cumbersome. Fortunately, we have found ways to study directly the asymptotic cases $c/m = 0$ and $c/m \rightarrow \infty$ corresponding to the special and ordinary transitions, respectively. Hence one gets back to single-mass problems. Nevertheless the technical problems that must be overcome to extend the calculations to higher orders of the loop expansion require considerably more effort than in the bulk case.

It is our hope that the present work might serve as a useful basis and starting point for further analyses that ultimately could lead to quantitative field-theory results for surface critical exponents and other universal quantities of a precision as good as in the bulk case. Finally, we would also like to express our hope that our work might spur further experimental work as well as simulations, the latter especially for higher spin dimensionalities.

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APPENDIX A: TWO-LOOP CALCULATIONS FOR THE SPECIAL TRANSITION

In this appendix some details of our two-loop calculations for the special transition will be presented.

1. Mass renormalization

Our starting point is the Feynman graph expansion of $[G^{(0,2)}(p)]^{-1}$ to two-loop order, as given by (5.3) and (5.7). A useful observation is that the term $C_3(p)$ in (5.7) can be combined with the one $\propto [C_1(p)]^2$ as

$$C_3(p) - \frac{[C_1(p)]^2}{\kappa_0 + c_0} = \text{---} \bigcirc \text{---} \text{---} \bigcirc \text{---} \text{---} \quad , \quad (\text{A1})$$

where the line labeled “D” represents the difference

$$\hat{G}(\mathbf{p}; z, z') - \frac{1}{c_0 + \kappa_0} e^{-\kappa_0(z+z')} , \quad (\text{A2})$$

which is nothing but the Dirichlet propagator

$$\hat{G}_D(\mathbf{p}; z, z') = \frac{1}{2\kappa_0} \left[e^{-\kappa_0|z-z'|} - e^{-\kappa_0(z+z')} \right] . \quad (\text{A3})$$

We now perform the mass renormalization. That is, we express the bare mass m_0 in terms of m and u_0 . For our choice of bulk normalization conditions made in Sec. III A, one has (see, e.g., Ref. [51])

$$m_0^2 = m^2 - \frac{n+2}{6} u_0 I_1(m^2) + \frac{n+2}{18} u_0^2 [I_2(m^2) - m^2 I_3(m^2)] + \mathcal{O}(u_0^3) , \quad (\text{A4})$$

where

$$I_1(m^2) = \int_{\mathbf{k}} \frac{1}{k^2 + m^2} , \quad (\text{A5})$$

$$I_2(m^2) \equiv I_2(0, m^2) , \quad (\text{A6})$$

and

$$I_3(m^2) \equiv \left. \frac{\partial}{\partial k^2} I_2(k^2, m^2) \right|_{k^2=0} \quad (\text{A7})$$

with

$$I_2(k^2, m^2) = \int_{\mathbf{k}_1} \int_{\mathbf{k}_2} \frac{1}{(k_1^2 + m^2)(k_2^2 + m^2)[(\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k})^2 + m^2]} \quad (\text{A8})$$

are familiar bulk Feynman integrals. Unlike I_1 and I_2 , the integral I_3 is finite in three dimensions,

$$I_3(m^2) = -\frac{2}{27} \left(\frac{1}{8\pi m} \right)^2 . \quad (\text{A9})$$

The factor $1/8\pi m$ may be identified as the value for $d = 3$ of the one-loop integral

$$D(m) = \int_{\mathbf{k}} \frac{1}{(k^2 + m^2)^2} \quad (\text{A10})$$

of the bulk vertex function $\tilde{\Gamma}_{\text{bulk}}^{(4)}(\{\mathbf{0}\})$. In the massive field-theory approach, it is common to absorb this factor in a properly defined renormalized coupling constant. We did this when introducing the rescaled renormalized coupling constant \tilde{u} via (5.8). (Note that the rescaling factor $b_n(d)$ in this equation becomes $[6/(n+8)]8\pi$ when $d = 3$.)

So far (namely, in (A1) as well as in the main text) we used the convention that the lines in Feynman graphs represent the free and reduced propagators (2.6) and (5.6), respectively. For the purpose of determining the results of the mass renormalization, it is preferable to use a different one in which the full and dashed propagator lines denote the modified expressions one obtains from the previous ones through the replacement $m_0^2 \rightarrow m^2$, i.e., of κ_0 by $\kappa = \sqrt{p^2 + m^2}$.

Let us decompose \hat{G} into its bulk part

$$\hat{G}_b(\mathbf{p}; z, z') = \frac{1}{2\kappa} e^{-\kappa|z-z'|} \quad (\text{A11})$$

and its surface part

$$\hat{G}_s(\mathbf{p}; z, z') = \frac{1}{2\kappa} \frac{\kappa - c_0}{\kappa + c_0} e^{-\kappa(z+z')} , \quad (\text{A12})$$

writing

$$\hat{G}(\mathbf{p}; z, z') = \hat{G}_b(\mathbf{p}; z, z') + \hat{G}_s(\mathbf{p}; z, z') , \quad (\text{A13})$$

and label lines representing \hat{G}_b and \hat{G}_s by “b” and “s”, respectively. Since the term linear in u_0 in (A4) is given by the Feynman diagram



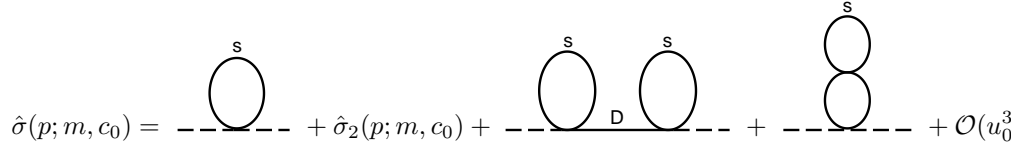
$$, \quad (\text{A14})$$

it is clear that the perturbative corrections originating from this term provide subtractions for the tadpole subgraphs such that only their surface part



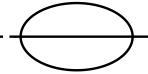
$$, \quad (\text{A15})$$

remains. Thus the self-energy $\hat{\sigma}$ introduced in (7.2) becomes



$$\hat{\sigma}(p; m, c_0) = \text{---} \text{---} \text{---} + \hat{\sigma}_2(p; m, c_0) + \text{---} \text{---} \text{---} + \text{---} \text{---} \text{---} + \mathcal{O}(u_0^3) \quad (\text{A16})$$

with



$$\hat{\sigma}_2(p; m, c_0) = \text{---} \text{---} \text{---} - \frac{1}{2\kappa} \frac{n+2}{18} u_0^2 [I_2(m^2) - m^2 I_3(m^2)] . \quad (\text{A17})$$

The latter combination, $\hat{\sigma}_2$, is uv finite for $d < 4$. However, the contributions of the other three graphs in (A16), which we shall denote as $\hat{\sigma}_1$, $\hat{\sigma}_3$, and $\hat{\sigma}_4$, respectively, are not because they still contain an uv divergence that must be absorbed through the renormalization of the surface enhancement.

2. Surface-enhancement renormalization

Upon substituting $\hat{G}^{(0,2)}$ from (7.2) into the normalization condition (5.1a), one is led to an equation for the shift δc introduced in (3.6):

$$\delta c = \left\{ [Z_1(c)Z_\phi]^{-1} - 1 \right\} (c + m) + \hat{\sigma}(0; m, c_0 = c + \delta c) . \quad (\text{A18})$$

This can be solved by iteration to determine the dependence of $c_0 = c + \delta c$ on c and m , order by order of perturbation theory in u_0 (or u). Using it (7.2) can be rewritten as

$$[\hat{G}^{(0,2)}(p)]^{-1} = \kappa - m + [Z_1(c)Z_\phi]^{-1} (c + m) - [\hat{\sigma}(p; m, c + \delta c) - \hat{\sigma}(0; m, c + \delta c)] . \quad (\text{A19})$$

Graphically the result can be interpreted as follows: To obtain $[\hat{G}^{(0,2)}(p)]^{-1}$ one can set $\delta c = 0$ if each graph of $\hat{\sigma}$ is taken to represent the graph itself subtracted by its value at $p = 0$ and the corresponding subtractions are also made for subgraphs involving lower-contributions to $\hat{\sigma}$. This is analogous to the familiar graphical interpretation of mass renormalization in the bulk vertex function $\tilde{\Gamma}^{(2)}(q)$ (see, e.g., [86]).

Let us be more specific in the special case $c = 0$. Upon setting $c = 0$ in (A18), we see that the $\mathcal{O}(u_0)$ term of the shift δc can be written as

$$\delta c^{(1)} = [(Z_1^{\text{sp}} Z_\phi)^{-1}]^{(1)} m + \hat{\sigma}_1(0; m, c_0 = 0) . \quad (\text{A20})$$

The $\mathcal{O}(u_0)$ term $[(Z_1^{\text{sp}} Z_\phi)^{-1}]^{(1)}$ will be calculated in the next subsection. The second contribution to $\delta c^{(1)}$ is uv singular for $d = 3$. It provides the singular part of the counterterm that cancels the uv divergence of $\hat{\sigma}_1(p; m, 0)$. To show this, let us calculate this quantity. We have

$$\begin{aligned}
\hat{\sigma}_1(p; m, 0) &= -\frac{u_0}{2} \frac{n+2}{3} \int_0^\infty dz e^{-2\kappa z} \int_{\mathbf{p}'} \frac{1}{2\kappa'} e^{-2\kappa' z} = -\frac{u_0}{8} \frac{n+2}{3} \int_{\mathbf{p}'} \frac{1}{(\kappa' + \kappa)\kappa'} \\
&= -\frac{u_0}{8} \frac{n+2}{3} m^{d-3} K_{d-1} J\left(\frac{p}{m}; d\right),
\end{aligned} \tag{A21}$$

with $K_d = 2^{1-d} \pi^{-d/2} / \Gamma(d/2)$, where

$$J(P; d) = \frac{1}{2} \int_0^\infty \frac{y^{(d-3)/2} dy}{(\sqrt{P^2+1} + \sqrt{y+1}) \sqrt{y+1}} = \int_0^\infty dy y^{(d-3)/2} \frac{d}{dy} \ln [\sqrt{P^2+1} + \sqrt{y+1}]. \tag{A22}$$

Subtracting from the latter integral its value at $P = 0$ yields the finite $d = 3$ expression

$$[J(P; d) - J(0; d)]_{d=3} = -\ln \frac{1 + \sqrt{P^2+1}}{2} = -\frac{1}{4} P^2 + \mathcal{O}(P^4). \tag{A23}$$

These results can be substituted into the Dyson form (7.2) of $\hat{G}^{(0,2)}$ to obtain

$$\left\{ \hat{G}^{(0,2)}[p; m, c_0(c=0, m)] \right\}^{-1} = \kappa + [(Z_1^{\text{sp}} Z_\phi)^{-1}]^{(1)} m - \frac{n+2}{3} \frac{u_0}{8\pi} \ln \frac{m+\kappa}{2m} + \mathcal{O}(u_0^2). \tag{A24}$$

At two-loop order, the first-order shift $\delta c^{(1)}$ must be taken into account in $\hat{\sigma}_1$. It produces an $\mathcal{O}(u_0^2)$ contribution of the form

$$\delta c^{(1)} \frac{\partial \hat{\sigma}_1}{\partial c_0}(p; m, c_0=0), \tag{A25}$$

whose uv singular part must remove the divergence of the tadpole subgraph (A15) of $\hat{\sigma}_4$. Since the same subgraph appears (twice) in $\hat{\sigma}_3$ one may be surprised at the apparent absence of the corresponding subtraction terms one obtains through replacement of one or both of these subgraphs by their singular parts¹⁶, and one may wonder whether $\hat{\sigma}_3$ be uv finite. In fact, the analog of $\hat{\sigma}_3$ that has the Dirichlet line “D” replaced by a full propagator line would need such subtractions, and those would occur, had we not reorganized the expansion in the manner of (A1) to obtain graphs whose internal vertices z and z' are connected by the Dirichlet propagator $\hat{G}_D(\mathbf{p}; z, z')$. The contribution $\hat{\sigma}_3$ is uv finite because \hat{G}_D vanishes whenever z or z' approach zero. Replacing one or both tadpoles (A15) in $\hat{\sigma}_3$ by their singular parts¹⁶ $\propto \delta(z)$ and $\propto \delta(z')$ would produce vanishing results.

According to (5.2a), we just need the expansion coefficients of order p^2 of $[\hat{G}^{(0,2)}(p)]^{-1}$ to determine $Z_1^{\text{sp}} Z_\phi$. Therefore we shall refrain from deriving the full two-loop result for $[\hat{G}^{(0,2)}(p)]^{-1}$ here. Before turning to the calculation of $Z_1^{\text{sp}} Z_\phi$, let us compute the derivative $\partial \hat{\sigma}_1 / \partial c_0$ in (A25). This is finite for $d = 3$, and its $\mathcal{O}(p^2)$ coefficient will be needed below. A straightforward calculation gives

$$\frac{\partial \hat{\sigma}_1}{\partial c_0}(p; m, c_0=0) = u_0 \frac{n+2}{12} \int_{\mathbf{p}'} \frac{1}{(\kappa' + \kappa)(\kappa')^2} = \frac{u_0}{8\pi m} \frac{n+2}{3} \frac{m}{m+\kappa} \ln \frac{m+\kappa}{m} \tag{A26}$$

$$= \frac{u_0}{8\pi m} \frac{n+2}{3} \left[\ln 2 + \frac{1}{4} (1 - \ln 4) \frac{p^2}{m^2} \right] + \mathcal{O}(p^4). \tag{A27}$$

3. Calculation of $Z_1^{\text{sp}} Z_\phi$

Using the representation (5.2a) of this renormalization factor, one can easily deduce from (A21) and (A23) its $\mathcal{O}(u_0)$ term:

¹⁶In the dimensionally regularized theory, the singular part of (A15) has the form $(d-3)^{-1} \delta(z)$; if one rather employs a cutoff regularization scheme, restricting the parallel momentum integrations by $p \leq \Lambda$, then the pole gets replaced by $\ln \Lambda$.

$$[(Z_1^{\text{sp}} Z_\phi)^{-1}]^{(1)} = -2m \left. \frac{\partial \hat{\sigma}_1(p; m, 0)}{\partial p^2} \right|_{p=0} = -\frac{n+2}{12} \frac{u_0}{8\pi m}. \quad (\text{A28})$$

The terms of order u_0^2 can be written as

$$[(Z_1^{\text{sp}} Z_\phi)^{-1}]^{(2)} = \left(\frac{n+2}{3} \frac{u_0}{8\pi m}\right)^2 \frac{1 - \ln 4}{8} - 2m \sum_{j=2}^4 \frac{\partial}{\partial p^2} \left[\hat{\sigma}_j(p; m, 0) + \delta_{j4} \hat{\sigma}_1(0; m, 0) \frac{\partial \hat{\sigma}_1(p; m, 0)}{\partial c_0} \right]_{p=0}. \quad (\text{A29})$$

The first term is the part of (A25) produced by the contribution $[(Z_1^{\text{sp}} Z_\phi)^{-1}]^{(1)}$ of the shift (A20); the remaining part of (A25) is the last term in the square brackets.

To compute the contribution of $\hat{\sigma}_2$, we start from

$$-\text{---}\text{---}\left(\text{circle}\right)\text{---}\text{---}\Big|_{c_0=0} = \frac{n+2}{18} u_0^2 \int_0^\infty dz \int_0^\infty dz' e^{-\kappa(z+z')} \int d^{d-1}r [G_N(\mathbf{x}, \mathbf{x}')]^3 e^{i\mathbf{p}\cdot\mathbf{r}}, \quad (\text{A30})$$

where $\mathbf{x} = (\mathbf{x}_{\parallel}, z)$, $\mathbf{x}' = (\mathbf{x}'_{\parallel}, z')$, $\mathbf{r} \equiv \mathbf{x}_{\parallel} - \mathbf{x}'_{\parallel}$, and G_N denotes the Neumann propagator. Introducing

$$R_{\pm} = \sqrt{r^2 + (z \pm z')^2}, \quad (\text{A31})$$

we can write the latter as

$$G_{\text{N}}(\boldsymbol{x}, \boldsymbol{x}') = G_{\text{b}}(R_-) + G_{\text{b}}(R_+) . \quad (\text{A32})$$

Since the term (A30) is not uv finite for $d = 3$, one must use the form of the bulk propagator for general values of d ,

$$G_{\text{b}}(x) = (2\pi)^{-\frac{d}{2}} \left(\frac{m}{x}\right)^{\frac{d}{2}-1} K_{\frac{d}{2}-1}(mx) \, , \quad (\text{A33})$$

rather than the simpler one for $d = 3$,

$$G_b(x) = \frac{e^{-mx}}{4\pi x} . \quad (\text{A34})$$

The derivative $\partial/\partial p^2|_0$ may then be performed under the integral sign. Recalling the definition (A17) of $\hat{\sigma}_2$, one thus arrives at

$$-2m \left. \frac{\partial \hat{\sigma}_2(p; m, 0)}{\partial p^2} \right|_{p=0} = \frac{n+2}{18} u_0^2 \left[\sum_{\lambda, \mu, \rho=\pm} \left(I^{\lambda\mu\rho} + \frac{m}{d-1} J^{\lambda\mu\rho} \right) - \frac{I_2(m^2)}{2m^2} + \frac{1}{2} I_3(m^2) \right], \quad (\text{A35})$$

where we have introduced the integrals

$$I^{\lambda\mu\rho} = \int_0^\infty dz \int_0^\infty dz' (z+z') e^{-m(z+z')} \int d^{d-1}r G_b(R_\lambda) G_b(R_\mu) G_b(R_\rho) \quad (\text{A36})$$

and

$$J^{\lambda\mu\rho} = \int_0^\infty dz \int_0^\infty dz' e^{-m(z+z')} \int d^{d-1}r r^2 G_b(R_\lambda) G_b(R_\mu) G_b(R_\rho) . \quad (\text{A37})$$

Owing to the bulk singularity contained in the distribution $[G_b(R_-)]^3$, I^{---} is not regular at $d = 3$. Its singularity must be canceled by that of the subtrahend $\propto I_2(m^2)$, a term which can be cast in the form

$$\frac{I_2(m^2)}{2m^2} = \frac{1}{m^2} \int_0^\infty dz \int d^{d-1}r [G_b(R)]^3 \quad (\text{A38})$$

with $R = \sqrt{r^2 + z^2}$. The symmetric double integral $\int_0^\infty dz \int_0^\infty dz'$ of I^{---} reduces to a single one, if we rewrite it as $\int_0^\infty dz_- \int_z^\infty dz_+$ with $z_\pm = z \pm z'$ and integrate over z_+ . This yields

$$I^{---} - \frac{I_2(m^2)}{2m^2} = \frac{1}{m^2} \int_0^\infty dz [(1 + mz)e^{-mz} - 1] \int d^{d-1}r [G_b(R)]^3. \quad (\text{A39})$$

We may now set $d = 3$ and perform the r integration. The result is

$$I^{---} - \frac{I_2(m^2)}{2m^2} = \frac{1}{32\pi^2 m^2} i^{---} \quad (\text{A40})$$

with

$$i^{---} = \int_0^\infty dz (e^{-mz} + mz e^{-mz} - 1) \left[\frac{e^{-3mz}}{z} - 3m E_1(3mz) \right], \quad (\text{A41a})$$

where $E_1(x)$ is the exponential integral function [54]. This can be evaluated with the help of the tables [87] and [88]. One gets

$$i^{---} = 2 - 7 \ln \frac{4}{3}. \quad (\text{A41b})$$

The remaining integrals in (A35) are uv finite for $d = 3$, so one can set $d = 3$ from the outset. A straightforward calculation gives

$$j^{---} \equiv 16\pi^2 m^3 J^{---} = -\frac{5}{6} + 3 \ln \frac{4}{3}, \quad (\text{A41c})$$

$$i^{+++} \equiv 32\pi^2 m^2 I^{+++} = \frac{7}{4} - 6 \ln \frac{4}{3}, \quad (\text{A41d})$$

and

$$j^{+++} \equiv 16\pi^2 m^3 J^{+++} = -\frac{31}{12} + 9 \ln \frac{4}{3}. \quad (\text{A41e})$$

The integrals $I^{\mp\pm\pm}$ and $J^{\mp\pm\pm}$ require a little more effort. Consider I^{-++} , for example. In the coordinates r , $x = (z - z')/r$, and $y = (z + z')/r$, the r integration becomes trivial, giving

$$\begin{aligned} i^{-++} \equiv 32\pi^2 m^2 I^{-++} &= m^2 \int_0^\infty dr \int_0^\infty dx \int_0^x dy \frac{rx}{\kappa_x^2 \kappa_y} e^{-mr(x+2\kappa_x+\kappa_y)} \\ &= \int_0^\infty dx \int_0^x dy \frac{x}{\kappa_x^2 \kappa_y (x + 2\kappa_x + \kappa_y)^2} \end{aligned} \quad (\text{A41f})$$

with $\kappa_x \equiv \sqrt{1+x^2}$. In a similar manner one derives

$$i^{+--} \equiv 32\pi^2 m^2 I^{+--} = \int_0^\infty dx \int_0^x dy \frac{x}{\kappa_x \kappa_y^2 (x + \kappa_x + 2\kappa_y)^2}, \quad (\text{A41g})$$

$$j^{-++} \equiv 16\pi^2 m^3 J^{-++} = \int_0^\infty dx \int_0^x dy \frac{1}{\kappa_x^2 \kappa_y (x + 2\kappa_x + \kappa_y)^3}, \quad (\text{A41h})$$

and

$$j^{+--} \equiv 16\pi^2 m^3 J^{+--} = \int_0^\infty dx \int_0^x dy \frac{1}{\kappa_x \kappa_y^2 (x + \kappa_x + 2\kappa_y)^3}. \quad (\text{A41i})$$

These integrals could be evaluated numerically in the present form. However, by making the familiar Euler substitutions, one can reduce the integrands to rational functions. Then the y integrations become standard and can be done exactly, so that one is left with single integrations over x . Finally, the latter can be transformed into integrations over the bounded interval $[0, 1]$, which is more convenient for numerical calculations. In Table XIII we have listed the numerical values of the integrals $i^{\mp\pm\pm}$ and $j^{\mp\pm\pm}$ together with those of the analytically known integrals i^{---} , j^{---} , i^{+++} , and j^{+++} .

TABLE XIII. Numerical values of the integrals $i^{\lambda\mu\rho}$ and $j^{\lambda\mu\rho}$ for $d = 3$.

$\lambda\mu\rho$	---	+-	-++	+++
$i^{\lambda\mu\rho}$	-0.0137745	0.1324282	0.0420126	0.0239076
$j^{\lambda\mu\rho}$	0.0297129	0.0114128	0.0075298	0.0058053

Substituting the above results and the value (A9) of I_3 into (A35) finally yields

$$-2m \left. \frac{\partial \hat{\sigma}_2(p; m, 0)}{\partial p^2} \right|_{p=0} = \frac{n+2}{3} \left(\frac{u_0}{8\pi m} \right)^2 A \quad (\text{A42a})$$

with

$$\begin{aligned} A &= \frac{1}{3} \sum_{\lambda, \mu, \rho=\pm} (i^{\lambda\mu\rho} + j^{\lambda\mu\rho}) - \frac{1}{162} \\ &= \frac{17}{162} - \frac{1}{3} \ln \frac{4}{3} + i^{+-} + i^{-++} + j^{+-} + j^{-++} \simeq 0.202428. \end{aligned} \quad (\text{A42b})$$

Next, consider $\hat{\sigma}_3$. Noting that the integrand is a symmetric function of z and z' , we find

$$\hat{\sigma}_3(p; m, 0) = \frac{1}{4} \left(\frac{n+2}{3} \frac{u_0}{8\pi} \right)^2 \frac{1}{\kappa} \int_0^\infty dz' \int_z^\infty dz \frac{e^{-2m(z+z')}}{zz'} e^{-2\kappa z'} (1 - e^{-\kappa z}). \quad (\text{A43})$$

The integrals one obtains upon performing the derivative $\partial/\partial p^2|_0$ can be worked out utilizing the mathematical tables [87–89]. This gives¹⁷

$$-2m \left. \frac{\partial \hat{\sigma}_3(p; m, 0)}{\partial p^2} \right|_{p=0} = \frac{1}{4} \left(\frac{n+2}{3} \frac{u_0}{8\pi m} \right)^2 \left[\text{Li}_2\left(-\frac{1}{2}\right) + \frac{\pi^2}{12} + \frac{1}{2} \ln \frac{2}{3} \right], \quad (\text{A44})$$

where $\text{Li}_2(x)$ is the polylogarithm of order 2 (see, e.g., Ref. [89]) with the value $\text{Li}_2(-\frac{1}{2}) = -0.4484142\dots$

It remains to compute the contribution of the combination $\hat{\sigma}_4 + \hat{\sigma}_1 \partial \hat{\sigma}_1 / \partial c_0$. The second term implies that from the term associated with the lower loop of $\hat{\sigma}_2$,

$$\frac{1}{2} \int_0^\infty \frac{dp' p'}{2\pi} \hat{G}_N^2(\mathbf{p}'; z, z'), \quad (\text{A45})$$

its value at $z' = 0$, multiplied by $e^{-2\kappa' z'}$ (the factor produced by the broken lines of $\hat{\sigma}_1$), gets subtracted. This entails that the contribution we are concerned with takes the form

$$-2m \left. \frac{\partial}{\partial p^2} \right|_{p=0} \left[\hat{\sigma}_4 + \hat{\sigma}_1 \frac{\partial \hat{\sigma}_1}{\partial c_0} \right] (p; m, 0) = \frac{1}{4} \left(\frac{n+2}{3} \frac{u_0}{8\pi m} \right)^2 g_4 \quad (\text{A46})$$

with

$$g_4 = \int_0^\infty dz \int_0^\infty dz' \frac{2z e^{-2(z+z')}}{z'} \left[F(z, z') - F(z, 0) e^{-2z'} \right], \quad (\text{A47})$$

where F denotes a sum of exponential integral functions [54]:

$$F(z, z') = \text{E}_1(2|z - z'|) + \text{E}_1(2z + 2z') + 2\text{E}_1(|z - z'| + z + z'). \quad (\text{A48})$$

The integrals contributing to g_4 can be evaluated analytically. One obtains

¹⁷Note that formula 3.1.3.2 on p. 567 of Ref. [87] is incorrect; its corrected form is given as 3.2.1.2 on p. 617 of Ref. [88].

$$g_4 = -\frac{\pi^2}{12} + \ln^2 2 + \frac{1}{2} \ln \frac{3}{2} - \text{Li}_2\left(-\frac{1}{2}\right). \quad (\text{A49})$$

Combining the above results yields

$$(Z_1^{\text{sp}} Z_\phi)^{-1} = 1 - \frac{n+2}{12} \frac{u_0}{8\pi m} + \frac{n+2}{3} \left[\frac{n+2}{12} \left(\frac{1}{2} - \ln 2 + \ln^2 2 \right) + A \right] \left(\frac{u_0}{8\pi m} \right)^2 + \mathcal{O}(u_0^3), \quad (\text{A50})$$

from which (5.17a) follows upon substitution of

$$\frac{u_0}{8\pi m} = \frac{6}{n+8} (\tilde{u} + \tilde{u}^2) + \mathcal{O}(\tilde{u}^3). \quad (\text{A51})$$

4. Calculation $Z_{\phi_s^2}^{\text{sp}}$

We start from the representation (5.2b) of this renormalization factor, perform the mass renormalization, and use (7.2) to express $[\hat{G}^{(0,2)}]^{-1}$ in terms of $\hat{\sigma}$, obtaining

$$(Z_{\phi_s^2}^{\text{sp}})^{-1} = Z_1^{\text{sp}} Z_\phi \left[1 - \frac{\partial \hat{\sigma}(0; m, c_0)}{\partial c_0} \right]_{c=0}. \quad (\text{A52})$$

Upon carrying out the surface-enhancement renormalization, we arrive at

$$\begin{aligned} Z_{\phi_s^2}^{\text{sp}} &= (Z_1^{\text{sp}} Z_\phi)^{-1} + \frac{n+2}{3} \frac{u_0}{8\pi m} \ln 2 + \left(\frac{n+2}{3} \frac{u_0}{8\pi m} \right)^2 \left(\frac{1}{2} - \frac{3}{4} \ln 2 + \ln^2 2 \right) \\ &+ \left[\hat{\sigma}_1(0; m, 0) \frac{\partial^2 \hat{\sigma}_1(0; m, c_0)}{\partial c_0^2} + \sum_{j=2}^4 \frac{\partial \hat{\sigma}_j(0; m, c_0)}{\partial c_0} \right]_{c_0=0} + \mathcal{O}(u_0^3) \end{aligned} \quad (\text{A53})$$

The explicitly given first $\mathcal{O}(u_0^2)$ contribution is the sum of the three terms $(\partial \hat{\sigma}_1 / \partial c_0)^2$, $-(Z_1^{\text{sp}} Z_\phi)^{(1)} \partial \hat{\sigma}_1 / \partial c_0$, and $-(Z_1^{\text{sp}} Z_\phi)^{(1)} m \partial^2 \hat{\sigma}_1 / \partial c_0^2$, whose last one is one part of the contribution proportional to the $\mathcal{O}(u_0)$ shift $\delta c^{(1)}$ (the other part being the contribution proportional to the uv singular tadpole graph $\hat{\sigma}_1$). The values of $(Z_1^{\text{sp}} Z_\phi)^{(1)}$ and $\partial \hat{\sigma}_1 / \partial c_0$ may be read off from (A50) and (A26), respectively; the required second derivative is

$$\frac{\partial^2 \hat{\sigma}_1}{\partial c_0^2}(0; m, c_0=0) = -u_0 \frac{n+2}{6} \int_{\mathbf{p}'} \frac{1}{(\kappa' + m)(\kappa')^3} = -\frac{n+2}{3} \frac{u_0}{4\pi m^2} (1 - \ln 2). \quad (\text{A54})$$

The remaining contributions in (A53) can be computed by proceeding along lines similar to those taken in our calculation of $Z_1^{\text{sp}} Z_\phi$. The contribution of $\hat{\sigma}_2$ is given by the derivative $\partial / \partial c_0$ of the graph (A30) at $c_0 = 0$. It can be written as

$$\frac{\partial \hat{\sigma}_2}{\partial c_0}(0; m, c_0=0) = -\frac{n+2}{3} \left(\frac{u_0}{8\pi m} \right)^2 B \quad (\text{A55a})$$

with

$$B = -\frac{(8\pi m)^2}{6} \int_0^\infty dz \int_0^\infty dz' e^{-m(z+z')} \int d^{d-1}r \frac{\partial}{\partial c_0} [G(\mathbf{x}, \mathbf{x}')]^3 \Big|_{c_0=0}, \quad (\text{A55b})$$

where again $\mathbf{r} = \mathbf{x}_\parallel - \mathbf{x}'_\parallel$. The required derivative $(\partial G^3 / \partial c_0)_{c_0=0} = 3G_N^2 (\partial G / \partial c_0)_{c_0=0}$ can be computed in the $\mathbf{p}z$ representation. Upon setting $d = 3$ and performing the angular integration, we find

$$\frac{\partial}{\partial c_0} G(\mathbf{x}, \mathbf{x}') \Big|_{c_0=0} = - \int_{\mathbf{p}} \frac{e^{-\kappa(z+z')}}{\kappa^2} e^{-i\mathbf{p} \cdot \mathbf{r}} = - \int_0^\infty \frac{dp p}{2\pi \kappa^2} J_0(pr) e^{-\kappa(z+z')}. \quad (\text{A56})$$

We insert this, together with the decomposition (A32) of G_N , into (A56) and perform the angular part of the integration $\int d^2r$. This yields

$$B = 2 \sum_{\lambda, \mu = \mp} k^{\lambda\mu} \quad (\text{A57})$$

with

$$k^{\lambda\mu} = m^2 \int_0^\infty dr r \int_0^\infty \frac{dp p}{\kappa^2} J_0(pr) \int_0^\infty dz \int_0^\infty dz' e^{-(\kappa+m)(z+z')} \frac{e^{-m(R_\lambda+R_\mu)}}{R_\lambda R_\mu}, \quad (\text{A58})$$

where $R_{\lambda=\mp}$ is defined by (A31).

Changing again to the variables $z_\pm = z \pm z'$, we can rewrite the symmetric double integrals $\int_0^\infty dz \int_0^\infty dz'$ in k^{--} and k^{++} as $\int_0^\infty dz_- \int_{z_-}^\infty dz_+$ and $\int_0^\infty dz_+ \int_0^{z_+} dz_-$, respectively. The inner one of these z integrations can now be performed to get

$$k^{\lambda\lambda} = m^2 \int_0^\infty dr r \int_0^\infty \frac{dp p}{\kappa^2} J_0(pr) \int_0^\infty dz \frac{e^{-(\kappa+m)z-2mR}}{R^2} \times \begin{cases} (\kappa+m)^{-1} & \text{for } \lambda = - , \\ z & \text{for } \lambda = + , \end{cases} \quad (\text{A59})$$

where $R = \sqrt{r^2 + z^2}$, as before. Next we make the variable transformation $r \rightarrow r/z$. Then the integrals over z simplify to

$$\int_0^\infty dz e^{-(\kappa+m+2mR)z} J_0(prz) \times \begin{cases} 1 & \text{for } \lambda = - , \\ z & \text{for } \lambda = + , \end{cases} \quad (\text{A60})$$

standard integrals, which can be found in tables [88]. In this manner one obtains

$$k^{--} = \int_0^\infty \frac{dr r}{\kappa_r^2} \int_0^\infty \frac{dp p}{\kappa_p^2 (\kappa_p + 1) \sqrt{(1 + \kappa_p + 2\kappa_r)^2 + (pr)^2}} \quad (\text{A61a})$$

and

$$k^{++} = \int_0^\infty \frac{dr r}{\kappa_r^2} \int_0^\infty \frac{dp p}{\kappa_p^2} \frac{1 + \kappa_p + 2\kappa_r}{\left[(1 + \kappa_p + 2\kappa_r)^2 + (pr)^2 \right]^{3/2}}, \quad (\text{A61b})$$

where as before $\kappa_p \equiv \sqrt{p^2 + 1}$. To compute these integrals, we had to resort once more to numerical means. Our results read

$$k^{--} = 0.1538951, \quad (\text{A62})$$

$$k^{++} = 0.0469337. \quad (\text{A63})$$

The “mixed” term k^{-+} is more complicated since its double z integration does not reduce to a single one. We first rescale z , z' , and r , so that $z/r \rightarrow z$, $z'/r \rightarrow z'$, and $mr \rightarrow r$. This leads us to

$$k^{-+} = \int_0^\infty dr r \int_0^\infty \frac{dp p}{\kappa_p^2} J_0(pr) \int_0^\infty dz \int_0^\infty dz' e^{-r(\kappa_p+1)(z+z')} \frac{e^{-r\sqrt{|z-z'|^2+1}}}{\sqrt{|z-z'|^2+1}} \frac{e^{-r\sqrt{(z+z')^2+1}}}{\sqrt{(z+z')^2+1}}. \quad (\text{A64})$$

The integral over r is of the form (A60) with $\lambda = +$ and hence can be calculated. Rewriting $\int_0^\infty dz \int_0^\infty dz'$ as $\int_0^\infty dy \int_0^y dx$ with $y = z + z'$ and $x = z - z'$ finally gives the representation we used to determine k^{-+} by numerical integration:

$$k^{-+} = \int_0^\infty \frac{dp p}{\kappa_p^2} \int_0^\infty \frac{dy}{\kappa_y} \int_0^y \frac{dx}{\kappa_x} \frac{\kappa_y + \kappa_x + (\kappa_p + 1)y}{\left\{ [\kappa_y + \kappa_x + (\kappa_p + 1)y]^2 + p^2 \right\}^{3/2}}. \quad (\text{A65})$$

Our result for k^{-+} is

$$k^{-+} \simeq 0.0691008. \quad (\text{A66})$$

In conjunction with (A62) it yields

$$B = 2 (k^{--} + 2k^{-+} + k^{++}) \simeq 0.678061, \quad (\text{A67})$$

which is the numerical value quoted in (5.20).

The other two-loop contributions to $Z_{\phi_s}^{\text{sp}}$ can be worked out analytically. Performing first the parallel-momentum loop integrations and thereafter the remaining ones over z and z' , one finds that¹⁸

$$\frac{\partial \hat{\sigma}_3}{\partial c_0}(0; m, 0) = \left(\frac{n+2}{3} \frac{u_0}{8\pi m} \right)^2 \left[\text{Li}_2\left(-\frac{1}{2}\right) + \frac{\pi^2}{12} + \frac{1}{2} \ln 2 - \frac{3}{4} \ln 3 \right] \quad (\text{A68})$$

and

$$\begin{aligned} \left(\frac{\partial \hat{\sigma}_4}{\partial c_0} + \hat{\sigma}_1 \frac{\partial^2 \hat{\sigma}_1}{\partial c_0^2} \right)(0; m, 0) &= \left(\frac{n+2}{3} \frac{u_0}{8\pi m} \right)^2 \left\{ \left[\frac{\pi^2}{24} - \frac{5}{2} \ln 2 + \frac{3}{4} \ln 3 \right] \right. \\ &\quad \left. + \left[-\text{Li}_2\left(-\frac{1}{2}\right) - \frac{\pi^2}{8} + \ln 2 + \frac{1}{4} \ln^2 2 \right] \right\} \\ &= \left(\frac{n+2}{3} \frac{u_0}{8\pi m} \right)^2 \left[\frac{3}{4} \ln \frac{3}{4} + \frac{1}{4} \ln^2 2 - \text{Li}_2\left(-\frac{1}{2}\right) - \frac{\pi^2}{12} \right]. \end{aligned} \quad (\text{A69})$$

In the first version of (A69), the term in the first pair of square brackets represents the part of $\partial \hat{\sigma}_4 / \partial c_0$ that results from the action of the derivative $\partial / \partial c_0$ on the tadpole subgraph (A15) of $\hat{\sigma}_4$ (by which an insertion of $\phi_s^2/2$ is produced there). Whereas this part is uv finite at $d = 3$, the other one (with an insertion of $\phi_s^2/2$ at the lower loop) must be combined with the remaining term $\propto \hat{\sigma}_1$ to obtain the finite result pertaining to the second pair of square brackets.

Combining these results yields

$$\begin{aligned} Z_{\phi_s}^{\text{sp}} &= 1 + \frac{n+2}{3} \frac{u_0}{8\pi m} \left(\ln 2 - \frac{1}{4} \right) \\ &\quad + \frac{n+2}{3} \left(\frac{u_0}{8\pi m} \right)^2 \left[A - B + \frac{n+2}{3} \left(\frac{1}{4} \ln^2 2 - \ln 2 \right) \right] + \mathcal{O}(u_0^3), \end{aligned} \quad (\text{A70})$$

from which (5.17b) follows by expressing u_0 in terms of \tilde{u} using (A51). Just as in the case of $Z_1^{\text{sp}} Z_\phi$, the number $\text{Li}_2(-1/2)$ has canceled out.

APPENDIX B: TWO-LOOP FEYNMAN DIAGRAMS FOR THE ORDINARY TRANSITION

We first show that the last two two-loop contributions in (A16), $\hat{\sigma}_3(p; m, c_0)$ and $\hat{\sigma}_4(p; m, c_0)$, sum to zero when $c_0 = \infty$:

$$\hat{\sigma}_3(p; m, \infty) + \hat{\sigma}_4(p; m, \infty) = \left[\text{Diagram 1} + \text{Diagram 2} \right]_{c_0=\infty} = 0. \quad (\text{B1})$$

(Note: Diagram 1 is a two-loop diagram with two internal lines labeled 's' and one external line labeled 'D'. Diagram 2 is a two-loop diagram with two internal lines labeled 's' and one external line labeled 'D'.)

A straightforward calculation gives

$$\hat{\sigma}_j(p; m, \infty) = \frac{u_0^2}{128} \left(\frac{n+2}{3} \right)^2 \int_{\mathbf{p}_1} \int_{\mathbf{p}_2} \frac{1}{\kappa_1 \kappa_2} L_j(\kappa, \kappa_1, \kappa_2), \quad j = 3, 4, \quad (\text{B2})$$

with

$$\begin{aligned} L_3(\kappa, \kappa_1, \kappa_2) &= \frac{4}{\kappa} \int_0^\infty dz \int_0^\infty dz' e^{-\kappa(z+z') - 2(\kappa_1 z + \kappa_2 z')} \left[e^{-\kappa|z-z'|} - e^{-\kappa(z+z')} \right] \\ &= \frac{1}{\kappa} \frac{1}{\kappa + \kappa_1 + \kappa_2} \left(\frac{1}{\kappa + \kappa_1} + \frac{1}{\kappa + \kappa_2} \right) - \frac{1}{\kappa} \frac{1}{\kappa + \kappa_1} \frac{1}{\kappa + \kappa_2}. \end{aligned} \quad (\text{B3})$$

¹⁸Again, the tables of integrals [88] were used; note that formula 2.5.11.11 is misprinted: the argument of the exponential function in the integrand should read $(c-b)x$ instead of $(b-c)x$.

and

$$\begin{aligned}
L_4(\kappa, \kappa_1, \kappa_2) &= -\frac{4}{\kappa_1} \int_0^\infty dz \int_0^\infty dz' e^{-2(\kappa z + \kappa_2 z')} \left(e^{-\kappa_1 |z - z'|} - e^{-\kappa_1 (z + z')} \right)^2 \\
&= \frac{1}{\kappa_1} \left[\left(\frac{-1}{\kappa + \kappa_2} + \frac{2}{\kappa + \kappa_1 + \kappa_2} \right) \left(\frac{1}{\kappa + \kappa_1} + \frac{1}{\kappa_1 + \kappa_2} \right) - \frac{1}{\kappa + \kappa_1} \frac{1}{\kappa + \kappa_2} \right].
\end{aligned} \tag{B4}$$

Adding these contributions yields

$$\sum_{j=3}^4 L_j(\kappa, \kappa_1, \kappa_2) = \frac{\kappa_1 - \kappa_2}{(\kappa + \kappa_1)(\kappa + \kappa_2)(\kappa + \kappa_1 + \kappa_2)(\kappa_1 + \kappa_2)}. \tag{B5}$$

Hence the integral $\int_{\mathbf{p}_1} \int_{\mathbf{p}_2}$ in (B2) is identically zero because of the antisymmetric form of its integrand.

Therefore the $\mathcal{O}(u_0^2)$ term of $Z_{1,\infty} Z_\phi$ is indeed entirely given by the contribution of the quantity $\hat{\sigma}_2(p; m, \infty)$ defined in (A17), as we asserted in (7.24). To compute it, we can proceed as in our calculation of its $c_0 = 0$ analog in Appendix A. This leads us to

$$-2m \left. \frac{\partial \hat{\sigma}_2(p; m, \infty)}{\partial p^2} \right|_{p=0} = \frac{n+2}{3} \left(\frac{u_0}{8\pi m} \right)^2 C \tag{B6}$$

with

$$C := \frac{1}{3} (i^{---} + j^{---} - i^{+++} - j^{+++}) - \frac{1}{162} + i^{-++} + j^{-++} - i^{+--} - j^{+--}. \tag{B7}$$

Here i^{---}, \dots, j^{+--} are the integrals introduced in (A41a)–(A41i). Using the analytical values given in these equations together with the numerical ones listed in Table XIII, one arrives at the form (7.25) of our results for $Z_{1,\infty} Z_\phi$ and C .

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